Supplementary Material

Predicting Enthalpy of Combustion using Machine Learning

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Table S1. Enthalpy of combustion for surrogates Edwards & Maurice, 2001 [17].

Surrogate	**S1**	**S2**	**S3**	**S4**	**S5**
Enthalpy of Combustion (BTU/lb)	**18700**	**18530**	**18580**	**18650**	**43.3**
Compounds	**Vol (%)**				
n-hexane	5.5	-	-	-	-
Cyclohexane	8	-	-	-	-
n-heptane	8	-	-	-	-
Methyl cyclohexane	8	-	7.5	-	20
Toluene	8	-	-	-	-
n-octane	8	-	-	-	-
n-nonane	10	-	-	-	-
Cyclooctane	8	-	6.6	-	-
n-decane	10	2.5	15.6	-	-
Decalin	5	11.5	-	-	-
Tetralin	1	9.5	5.6		5
n-dodecane	10	-	17.4	6	30
1-methyl naphthalene	0.5	-	5.2	-	-
n-tetradecane	10	-	11.2	-	-
iso-octane	-	-	6.5	-	10
m-xylene	-	-	6.9	-	15
Butyl benzene	-	-	5.5	-	-
1,2,4,5 tetramethyl benzene	-	-	5.5	-	-
Dodecane	-	25	-	-	-
1-methyl naphthalene	-	1.5	-	-	-
Hexadecane	-	-	6.5	-	-
n-undecane	-	-	-	4.7	-
n-pentylcyclohexane	-	11	-	-	-
1,3-diisopropylbenzene	-	3	-	-	-
1-phenyl hexane	-	5	-	-	-
n-tridecane	-	10	-	18.8	-
n-heptylcyclohexane	-	11	-	-	-
n-tetradecane	-	5	-	12.5	20
n-pentadecane	-	5	-	-	-
n-hexylcyclopentane	-	-	-	2.7	-
n-heptylcyclopentane	-	-	-	3.6	-
n-octyl cyclopentane	-	-	-	11.2	-

n-nonylcyclopentane	-	-	-	7.5	-
Bicycloparaffin 1	-	-	-	11.3	-
Bicycloparaffin 2	-	-	-	14.7	-
Pentamethyl benzene	-	-	-	1.3	-
Hexamethylbenzene	-	-	-	1.7	-
Dimethylnaphthalene	-	-	-	4	-
Total	100	100	100	100	100

Table S2. Enthalpy of combustion for surrogates Huber et al. (2009) [18].

Surrogates	**S6**	**S7**
Enthalpy of Combustion (MJ/mol)	**7.18**	**7.23**
Compound	**Mol (%)**	
R-methyldecalin	35.4	35.4
5-methylnonane	15	8.4
2,4-dimethylnonane	0	7.1
n-dodecane	18.3	15.8
heptylcyclohexane	31.3	33.3
Total	100	100

Table S3. Enthalpy of combustion for surrogates Shrestha (2014) [19].

Surrogates	**S8**	**S9**	**S10**	**S11**	**S12**	**S13**
Enthalpy of Combustion (MJ/kg)	**43.19**	**43.16**	**43.18**	**43.11**	**43.30**	**43.31**
Compound	**Vol (%)**					
n-dodecane	58.0	60.0	56.0	56.0	51.0	51.0
iso-Cetane	-	-	-	-	9.0	11.0
Decalin	-	-	11.0	13.0	28.0	25.0
n-Propylbenzene	42.0	-	33.0	-	12.0	-
1,2,4-trimethylbenzene	-	40.0	-	31.0	-	13.0
Total	100	100	100	100	100	100

Table S4. Enthalpy of combustion for surrogates Kalghatgi et al. (2011) [20].

Surrogates	**S14**	**S15**	**S16**
Enthalpy of Combustion (MJ/kg)	**44.4**	**41.7**	**43.2**
Compound	**Vol (%)**		
Iso-octane	84.0	-	50.0
n-heptane	16.0	35.0	24.0
Toluene	-	65.0	26.0
Total	100	100	100

Table S5. Enthalpy of combustion for surrogates Huber et al. (2010) [21].

Surrogates	**S17**	**S18**
Enthalpy of Combustion (MJ/mol)	**6.55**	**6.76**
Compound	**Mol (%)**	
n-hexylcyclohexane	-	26.8
n-heptylcyclohexane	27.9	-
1-methyldecalin	1.3	6.4
5-methylnonane	16.5	13.0
2-methyldecane	15.4	28.4

n-tetradecane	5.7	3.5
n-hexadecane	3.3	-
ortho-xylene	7.1	9.4
Tetralin	22.8	12.5
Total	100	100

Table S6. Enthalpy of combustion for surrogates Eddings et al. (2005) [22].

Surrogates	**S19**	**S20**
Enthalpy of Combustion (MJ/kg)	**44.5**	**44.6**
Compound	**Mol (%)**	
n-octane	3.5	3.0
n-dodecane	40.0	30.0
n-hexadecane	5.0	12.0
Xylene	8.5	15.0
Tetralin	8.0	13.0
Decalin	35.0	27.0
Total	100	100

Table S7. Enthalpy of combustion for surrogates Naik et al. (2010) [23].

Surrogates	**S21**	**S22**
Enthalpy of Combustion (MJ/kg)	**44.55**	**44.45**
Compounds	**Mol (%)**	
iso-Octane	28.0	33.0
n-octane	61.0	25.0
n-dodecane	11.0	42.0
Total	100.0	100.0

Table S8. Enthalpy of combustion for surrogates Grubinger et al. (2021) [24].

Surrogates	**S23**	**S24**	**S25**
Enthalpy of Combustion (MJ/kg)	**44.79**	**43.32**	**41.4**
Compounds	**Mol (%)**		
n-butane	6.46	-	-
iso-pentane	17.50	-	32.78
1-pentene	-	15.77	-
n-hexane	21.08	22.89	-
Ethanol	-	-	10.01
Cyclohexane	-	-	18.69
iso-octane	43.85	13.88	8.20
Toluene	-	10.71	-
m-Xylene	8.57	29.02	24.75
t-decalin	2.55	-	5.58
n-pentylbenzene	-	7.73	-
Total	100	100	100

Table S9. Enthalpy of combustion for surrogates Xu et al. (2015) [25].

Surrogate	**S26**	**S27**	**S28**	**S29**	**S30**	**S31**	**S32**	**S33**	**S34**
Enthalpy of Combustion (MJ/kg)	**43.17**	**43.12**	**42.94**	**43.90**	**43.46**	**43.22**	**43.79**	**42.98**	**43.30**
Compound	**Mol (%)**								
1,2,4-trimethylbenzene	16.40	23.42	27.35	-	28.45	19.85	-	34.38	-
iso-undecane	37.33	-	-	-	-	-	24.70	-	-
n-undecane	25.22	19.33	-	-	-	-	-	-	-
butyl-cyclohexane	21.05	-	-	-	-	-	-	-	-
iso-dodecane	-	26.09	-	86.49	-	-	43.85	-	16.18
pentyl-cyclohexane	-	31.16	-	-	-	-	-	-	-
iso-tridecane	-	-	15.71	-	-	-	-	-	-
n-dodecane	-	-	13.02	-	-	9.44	-	-	-
hexylcyclohexane	-	-	29.72	-	-	-	-	-	60.73
methyl-dicyclohexane	-	-	14.21	-	-	22.43	-	-	-
iso-hexadecane	-	-	-	13.51	-	-	4.88	-	-
iso-tetradecane	-	-	-	-	71.55	-	-	-	-
iso-pentadecane	-	-	-	-	-	37.56	-	-	-
dicyclohexane	-	-	-	-	-	10.72	-	-	23.09
iso-nonane	-	-	-	-	-	-	8.72	-	-
iso-denane	-	-	-	-	-	-	17.85	48.90	-
n-denane	-	-	-	-	-	-	-	16.72	-
Total	100	100	100	100	100	100	100	100	100

Table S10. Enthalpy of combustion for surrogates Grubinger et al. (2021) [24].

Surrogate	**S35**	**S36**	**S37**	**S38**
Enthalpy of Combustion (MJ/kg)	**32.6**	**30.5**	**28.7**	**43.9**
Compounds	**Vol (%)**			
1,1,3,3 tetraethoxy-propane	70.0	-	-	-
2,2,4,4,6,8,8 heptamethyl-nonane	30.0	20.0	-	23.5
tri-propylene-glycol-methyl-ether	-	80.0	-	-
dibutyl-maleate	-	-	88.0	-
normal hexadecane	-	-	7.0	76.5
2-ethylhexyl-nitrate	-	-	5.0	-
Total	100	100	100	100