1,3,8-Trimethylnaphthalene

Inchi: InChI=1S/C13H14/c1-9-7-11(3)13-10(2)5-4-6-12(13)8-9/h4-8H,1-3H3
InchiKey: XYTKCJHHXQVFCK-UHFFFAOYSA-N
Formula: C13H14
SMILES: Cc1cc(C)c2c(C)cccc2c1
Mol. weight [g/mol]: 170.25
CAS: 17057-91-9

Physical Properties

Property code	Value	Unit	Source
gf	248.75	kJ/mol	Joback Method
hf	81.54	kJ/mol	Joback Method
hfus	19.32	kJ/mol	Joback Method
hvap	50.43	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	3.765		Crippen Method
mcvol	150.810	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
rinpol	261.68		NIST Webbook
rinpol	261.68		NIST Webbook
tb	557.44	K	Joback Method
tc	785.77	K	Joback Method
tf	332.95	K	Joback Method
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.00	J/mol×K	557.44	Joback Method
cpg	409.52	J/mol×K	747.71	Joback Method
cpg	397.73	J/mol×K	709.66	Joback Method
cpg	385.15	J/mol×K	671.60	Joback Method
cpg	371.70	J/mol×K	633.55	Joback Method
cpg	357.34	J/mol×K	595.49	Joback Method
cpg	420.56	J/mol×K	785.77	Joback Method

dvisc	0.0002834	Pa×s	557.44	Joback Method
dvisc	0.0003273	Pa×s	520.03	Joback Method
dvisc	0.0003866	Pa×s	482.61	Joback Method
dvisc	0.0004696	Pa×s	445.20	Joback Method
dvisc	0.0005911	Pa×s	407.78	Joback Method
dvisc	0.0007795	Pa×s	370.37	Joback Method
dvisc	0.0010939	Pa×s	332.95	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.70870e+01
Coeff. B	-6.76700e+03
Coeff. C	-3.39000e-01
Temperature range (K), min.	403.15
Temperature range (K), max.	575.00

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17057919&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume