Naphthalene, 1,3,5-trimethyl-

Other names: 1,3,5-trimethyl-naphthalene
Inchi: InChI=1S/C13H14/c1-9-7-11(3)12-6-4-5-10(2)13(12)8-9/h4-8H,1-3H3
InchiKey: IJEBSXFVVHGNQF-UHFFFAOYSA-N
Formula: C13H14
SMILES: Cc1cc(C)c2cccc(C)c2c1
Mol. weight [g/mol]: 170.25
CAS: 2131-39-7

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	262.72		NIST Webbook
rinpol	262.70		NIST Webbook
rinpol	262.70		NIST Webbook
rinpol	264.30		NIST Webbook
rinpol	264.30		NIST Webbook
rinpol	1578.00		NIST Webbook
rinpol	264.70		NIST Webbook
rinpol	264.00		NIST Webbook
ripol	2183.00		NIST Webbook
tb	557.70 ± 3.00	K	NIST Webbook
tc	785.77	K	Joback Method
tf	318.65 ± 0.60	K	NIST Webbook
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	357.34	J/mol×K	595.49	Joback Method
cpg	371.70	J/mol×K	633.55	Joback Method
cpg	385.15	J/mol×K	671.60	Joback Method
cpg	397.73	J/mol×K	709.66	Joback Method
cpg	409.52	J/mol×K	747.71	Joback Method
cpg	420.56	J/mol×K	785.77	Joback Method
dvisc	0.0010939	Pa×s	332.95	Joback Method
dvisc	0.0007795	Pa×s	370.37	Joback Method
dvisc	0.0005911	Pa×s	407.78	Joback Method
dvisc	0.0004696	Pa×s	445.20	Joback Method
dvisc	0.0003866	Pa×s	482.61	Joback Method
dvisc	0.0003273	Pa×s	520.03	Joback Method
dvisc	0.0002834	Pa×s	557.44	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2131397&Units=SI
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

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
rinpol: Non-polar retention indices
ripol: Polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume