Naphthalene, 1,2,3-trichloro

Other names: 1,2,3-trichloronaphthalene
naphthalene, 1,2,3-trichloro-
Inchi: InChI=1S/C10H5Cl3/c11-8-5-6-3-1-2-4-7(6)9(12)10(8)13/h1-5H
InchiKey: QEPTXDCPBXMWJC-UHFFFAOYSA-N
Formula: C10H5Cl3
SMILES: Clc1cc2ccccc2c(Cl)c1Cl
Mol. weight [g/mol]: 231.51

Physical Properties

Property code	Value	Unit	Source
gf	187.70	kJ/mol	Joback Method
hf	96.24	kJ/mol	Joback Method
hfus	18.44	kJ/mol	Evaluation of entropies of fusion of polychlorinated naphthalenes by model congeners: A DSC study
hvap	56.91	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.800		Crippen Method
mcvol	145.260	ml/mol	McGowan Method
pc	3235.66	kPa	Joback Method
rinpol	1827.00		NIST Webbook
rinpol	1827.00		NIST Webbook
rinpol	1827.00		NIST Webbook
tb	601.09	K	Joback Method
tc	855.98	K	Joback Method
tf	388.90	K	Joback Method
vc	0.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.79	J/mol×K	601.09	Joback Method
cpg	317.08	J/mol×K	813.50	Joback Method
cpg	310.35	J/mol×K	771.02	Joback Method

cpg	303.03	J/mol×K	728.54	Joback Method
cpg	295.05	J/mol×K	686.05	Joback Method
cpg	286.33	J/mol×K	643.57	Joback Method
cpg	323.30	J/mol×K	855.98	Joback Method
dvisc	0.0003683	Pa×s	601.09	Joback Method
dvisc	0.0004237	Pa×s	565.73	Joback Method
dvisc	0.0004967	Pa×s	530.36	Joback Method
dvisc	0.0005956	Pa×s	495.00	Joback Method
dvisc	0.0007344	Pa×s	459.63	Joback Method
dvisc	0.0009378	Pa×s	424.27	Joback Method
dvisc	0.0012520	Pa×s	388.90	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Evaluation of entropies of fusion of polychlorinated naphthalenes by model congeners? A DSC study:	https://www.doi.org/10.1016/j.tca.2006.04.011
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=R128580&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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