Naphthalene, 1,2,3,7,8-pentachloro

Other names: 1,2,3,7,8-pentachloronaphthalene
naphthalene, 1,2,3,7,8-pentachloro-
Inchi: InChI=1S/C10H3Cl5/c11-5-2-1-4-3-6(12)9(14)10(15)7(4)8(5)13/h1-3H
InchiKey: BFRRJXVSQTZQHM-UHFFFAOYSA-N
Formula: C10H3Cl5
SMILES: Clc1cc2ccc(Cl)c(Cl)c2c(Cl)c1Cl
Mol. weight [g/mol]: 300.40

Physical Properties

Property code	Value	Unit	Source
gf	144.58	kJ/mol	Joback Method
hf	41.82	kJ/mol	Joback Method
hfus	17.55	kJ/mol	Evaluation of entropies of fusion of polychlorinated naphthalenes by model congeners: A DSC study
hvap	67.00	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	6.107		Crippen Method
mcvol	169.740	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
rinpol	2309.00		NIST Webbook
rinpol	2309.00		NIST Webbook
rinpol	2309.00		NIST Webbook
tb	685.91	K	Joback Method
tc	947.92	K	Joback Method
tf	473.78	K	Joback Method
vc	0.654	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.73	J/mol×K	685.91	Joback Method
cpg	341.68	J/mol×K	904.25	Joback Method
cpg	336.44	J/mol×K	860.58	Joback Method

cpg	330.79	J/mol×K	816.91	Joback Method
cpg	324.67	J/mol×K	773.25	Joback Method
cpg	318.01	J/mol×K	729.58	Joback Method
cpg	346.58	J/mol×K	947.92	Joback Method
dvisc	0.0003445	Pa×s	685.91	Joback Method
dvisc	0.0003907	Pa×s	650.56	Joback Method
dvisc	0.0004495	Pa×s	615.20	Joback Method
dvisc	0.0005262	Pa×s	579.85	Joback Method
dvisc	0.0006286	Pa×s	544.49	Joback Method
dvisc	0.0007697	Pa×s	509.14	Joback Method
dvisc	0.0009715	Pa×s	473.78	Joback Method

Sources

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=R128555&Units=SI

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

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

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