

Naphthalene, 1,2,3,6,7-pentachloro

Other names:	1,2,3,6,7-pentachloronaphthalene naphthalene, 1,2,3,6,7-pentachloro-
Inchi:	InChI=1S/C10H3Cl5/c11-6-1-4-2-8(13)10(15)9(14)5(4)3-7(6)12/h1-3H
InchiKey:	MKCASBPThPJCDC-UHFFFAOYSA-N
Formula:	C10H3Cl5
SMILES:	Clc1cc2cc(Cl)c(Cl)c(Cl)c2cc1Cl
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	22.94	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	2217.00		NIST Webbook
rinpol	2217.00		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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R128520&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Evaluation of entropies of fusion of polychlorinated naphthalenes by model	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

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

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