

Naphthalene, 1,2,4,6,7-pentachloro

Other names:	1,2,4,6,7-pentachloronaphthalene naphthalene, 1,2,4,6,7-pentachloro-
Inchi:	InChI=1S/C10H3Cl5/c11-6-3-9(14)10(15)5-2-8(13)7(12)1-4(5)6/h1-3H
InchiKey:	GXQUDLBNLKOIQB-UHFFFAOYSA-N
Formula:	C10H3Cl5
SMILES:	Clc1cc2c(Cl)cc(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	22.58	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	2145.00		NIST Webbook
rinpol	2145.00		NIST Webbook
tb	685.91	K	Joback Method
tc	947.92	K	Joback Method
tf	473.78	K	Joback Method
vc	0.654	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.73	J/mol×K	685.91	Joback Method
cpg	318.01	J/mol×K	729.58	Joback Method
cpg	324.67	J/mol×K	773.25	Joback Method
cpg	330.79	J/mol×K	816.91	Joback Method

cpg	336.44	J/molxK	860.58	Joback Method
cpg	341.68	J/molxK	904.25	Joback Method
cpg	346.58	J/molxK	947.92	Joback Method
dvisc	0.0009715	Paxs	473.78	Joback Method
dvisc	0.0007697	Paxs	509.14	Joback Method
dvisc	0.0006286	Paxs	544.49	Joback Method
dvisc	0.0005262	Paxs	579.85	Joback Method
dvisc	0.0004495	Paxs	615.20	Joback Method
dvisc	0.0003907	Paxs	650.56	Joback Method
dvisc	0.0003445	Paxs	685.91	Joback Method

Sources

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 Joback Method 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=R128659&Units=SI

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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