

Naphthalene, 1,2,4,5,6,8-hexachloro

Other names:	1,2,4,5,6,8-hexachloronaphthalene naphthalene, 1,2,4,5,6,8-hexachloro-
Inchi:	InChI=1S/C10H2Cl6/c11-3-1-5(13)9(15)8-4(12)2-6(14)10(16)7(3)8/h1-2H
InchiKey:	JHKLUFTHIWTX-UHFFFAOYSA-N
Formula:	C10H2Cl6
SMILES:	Clc1cc(Cl)c2c(Cl)c(Cl)cc(Cl)c2c1Cl
Mol. weight [g/mol]:	334.84

Physical Properties

Property code	Value	Unit	Source
gf	123.02	kJ/mol	Joback Method
hf	14.61	kJ/mol	Joback Method
hfus	28.89	kJ/mol	Evaluation of entropies of fusion of polychlorinated naphthalenes by model congeners: A DSC study
hvap	72.05	kJ/mol	Joback Method
log10ws	-7.39		Crippen Method
logp	6.760		Crippen Method
mcvol	181.980	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
rinpol	2425.00		NIST Webbook
rinpol	2425.00		NIST Webbook
rinpol	2425.00		NIST Webbook
tb	728.32	K	Joback Method
tc	992.99	K	Joback Method
tf	516.22	K	Joback Method
vc	0.704	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.21	J/mol×K	728.32	Joback Method
cpg	331.53	J/mol×K	772.43	Joback Method
cpg	337.34	J/mol×K	816.54	Joback Method

cpg	342.69	J/molxK	860.66	Joback Method
cpg	347.65	J/molxK	904.77	Joback Method
cpg	352.28	J/molxK	948.88	Joback Method
cpg	356.64	J/molxK	992.99	Joback Method
dvisc	0.0008492	Paxs	516.22	Joback Method
dvisc	0.0006870	Paxs	551.57	Joback Method
dvisc	0.0005701	Paxs	586.92	Joback Method
dvisc	0.0004832	Paxs	622.27	Joback Method
dvisc	0.0004169	Paxs	657.62	Joback Method
dvisc	0.0003651	Paxs	692.97	Joback Method
dvisc	0.0003240	Paxs	728.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R128595&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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 PSC study:	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
mccol:	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

Latest version available from:

<https://www.cheméo.com/cid/77-005-1/Naphthalene-1-2-4-5-6-8-hexachloro.pdf>

Generated by Cheméo on 2024-04-28 09:36:04.792810951 +0000 UTC m=+16586213.713388272.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.