

Naphthalene, 1,3,5,7-tetrachloro-

Other names:	1,3,5,7-tetrachloronaphthalene
Inchi:	InChI=1S/C10H4Cl4/c11-5-1-7-8(10(14)3-5)2-6(12)4-9(7)13/h1-4H
InchiKey:	OTTCXKPQKOLSJN-UHFFFAOYSA-N
Formula:	C10H4Cl4
SMILES:	Clc1cc(Cl)c2cc(Cl)cc(Cl)c2c1
Mol. weight [g/mol]:	265.95
CAS:	53555-64-9

Physical Properties

Property code	Value	Unit	Source
gf	166.14	kJ/mol	Joback Method
hf	69.03	kJ/mol	Joback Method
hfus	27.14	kJ/mol	Evaluation of entropies of fusion of polychlorinated naphthalenes by model congeners: A DSC study
hvap	61.96	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.453		Crippen Method
mcvol	157.500	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
tb	643.50	K	Joback Method
tc	902.29	K	Joback Method
tf	431.34	K	Joback Method
vc	0.606	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.67	J/mol×K	643.50	Joback Method
cpg	330.01	J/mol×K	859.16	Joback Method
cpg	324.07	J/mol×K	816.03	Joback Method
cpg	317.64	J/mol×K	772.89	Joback Method
cpg	310.64	J/mol×K	729.76	Joback Method
cpg	303.01	J/mol×K	686.63	Joback Method

cpg	335.52	J/mol×K	902.29	Joback Method
dvisc	0.0003601	Paxs	643.50	Joback Method
dvisc	0.0004112	Paxs	608.14	Joback Method
dvisc	0.0004772	Paxs	572.78	Joback Method
dvisc	0.0005649	Paxs	537.42	Joback Method
dvisc	0.0006848	Paxs	502.06	Joback Method
dvisc	0.0008546	Paxs	466.70	Joback Method
dvisc	0.0011060	Paxs	431.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53555649&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 DSC study:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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