

Naphthalene, 1,4,5-trichloro

Inchi:	InChI=1S/C10H5Cl3/c11-7-4-5-9(13)10-6(7)2-1-3-8(10)12/h1-5H
InchiKey:	VQSNXLCFFHGXTI-UHFFFAOYSA-N
Formula:	C10H5Cl3
SMILES:	Clc1ccc(Cl)c2c(Cl)cccc12
Mol. weight [g/mol]:	231.51

Physical Properties

Property code	Value	Unit	Source
gf	187.70	kJ/mol	Joback Method
hf	96.24	kJ/mol	Joback Method
hfus	24.14	kJ/mol	Joback Method
hvap	56.91	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.800		Crippen Method
mcvol	145.260	ml/mol	McGowan Method
pc	3235.66	kPa	Joback Method
rinpol	1852.00		NIST Webbook
rinpol	1852.00		NIST Webbook
tb	601.09	K	Joback Method
tc	855.98	K	Joback Method
tf	388.90	K	Joback Method
vc	0.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.79	J/molxK	601.09	Joback Method
cpg	317.08	J/molxK	813.50	Joback Method
cpg	310.35	J/molxK	771.02	Joback Method
cpg	303.03	J/molxK	728.54	Joback Method
cpg	295.05	J/molxK	686.05	Joback Method
cpg	286.33	J/molxK	643.57	Joback Method
cpg	323.30	J/molxK	855.98	Joback Method
dvisc	0.0003683	Paxs	601.09	Joback Method

dvisc	0.0004237	Paxs	565.73	Joback Method
dvisc	0.0004967	Paxs	530.36	Joback Method
dvisc	0.0005956	Paxs	495.00	Joback Method
dvisc	0.0007344	Paxs	459.63	Joback Method
dvisc	0.0009378	Paxs	424.27	Joback Method
dvisc	0.0012520	Paxs	388.90	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=R128897&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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