

1,2,4-Trichloro-5-(cyclohexyloxy)benzene

Inchi:	InChI=1S/C12H13Cl3O/c13-9-6-11(15)12(7-10(9)14)16-8-4-2-1-3-5-8/h6-8H,1-5H2
InchiKey:	PVPGPRLXAYPWIL-UHFFFAOYSA-N
Formula:	C12H13Cl3O
SMILES:	Clc1cc(Cl)c(OC2CCCCC2)cc1Cl
Mol. weight [g/mol]:	279.59
CAS:	116401-37-7

Physical Properties

Property code	Value	Unit	Source
gf	17.34	kJ/mol	Joback Method
hf	-214.01	kJ/mol	Joback Method
hfus	25.32	kJ/mol	Joback Method
hvap	62.56	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	5.358		Crippen Method
mcvol	187.910	ml/mol	McGowan Method
pc	2482.59	kPa	Joback Method
tb	669.84	K	Joback Method
tc	920.41	K	Joback Method
tf	408.35	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.72	J/molxK	669.84	Joback Method
cpg	461.60	J/molxK	711.60	Joback Method
cpg	476.25	J/molxK	753.36	Joback Method
cpg	489.70	J/molxK	795.12	Joback Method
cpg	501.97	J/molxK	836.89	Joback Method
cpg	513.09	J/molxK	878.65	Joback Method
cpg	523.10	J/molxK	920.41	Joback Method
dvisc	0.0011169	Paxs	408.35	Joback Method
dvisc	0.0006834	Paxs	451.93	Joback Method

dvisc	0.0004558	Paxs	495.51	Joback Method
dvisc	0.0003247	Paxs	539.10	Joback Method
dvisc	0.0002433	Paxs	582.68	Joback Method
dvisc	0.0001897	Paxs	626.26	Joback Method
dvisc	0.0001529	Paxs	669.84	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=C116401377&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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