Clofoctol, methyl ether

Inchi: InChI=1S/C22H28Cl2O/c1-21(2,3)14-22(4,5)17-8-10-20(25-6)16(12-17)11-15-7-9-18(23)
InchiKey: WCOGVAKQAAUJCO-UHFFFAOYSA-N
Formula: C22H28Cl2O
SMILES: COc1ccc(C(C)(C)CC(C)(C)C)cc1Cc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 379.36

Physical Properties

Property code	Value	Unit	Source
gf	197.48	kJ/mol	Joback Method
hf	-251.43	kJ/mol	Joback Method
hfus	34.02	kJ/mol	Joback Method
hvap	80.35	kJ/mol	Joback Method
log10ws	-7.81		Crippen Method
logp	7.307		Crippen Method
mcvol	303.670	ml/mol	McGowan Method
pc	1293.00	kPa	Joback Method
rinpol	2523.80		NIST Webbook
rinpol	2523.80		NIST Webbook
tb	866.86	K	Joback Method
tc	1102.08	K	Joback Method
tf	527.53	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	890.76	J/mol×K	866.86	Joback Method
cpg	907.58	J/mol×K	906.06	Joback Method
cpg	923.17	J/mol×K	945.27	Joback Method
cpg	937.64	J/mol×K	984.47	Joback Method
cpg	951.11	J/mol×K	1023.68	Joback Method
cpg	963.67	J/mol×K	1062.88	Joback Method
cpg	975.46	J/mol×K	1102.08	Joback Method
dvisc	0.0003130	Pa×s	527.53	Joback Method

dvisc	0.0001743	Pa×s	584.08	Joback Method
dvisc	0.0001076	Pa×s	640.64	Joback Method
dvisc	0.0000719	Pa×s	697.19	Joback Method
dvisc	0.0000510	Pa×s	753.75	Joback Method
dvisc	0.0000380	Pa×s	810.30	Joback Method
dvisc	0.0000294	Pa×s	866.86	Joback Method

Sources

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=U333470&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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