Hexadecyl dichloroacetate

Inchi: InChI=1S/C18H34Cl2O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-22-18(21)17(19)20/h1
InchiKey: WDSYEOLRIOORQD-UHFFFAOYSA-N
Formula: C18H34Cl2O2
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(Cl)Cl
Mol. weight [g/mol]: 353.37

Physical Properties

Property code	Value	Unit	Source
gf	-159.54	kJ/mol	Joback Method
hf	-696.41	kJ/mol	Joback Method
hfus	50.03	kJ/mol	Joback Method
hvap	73.20	kJ/mol	Joback Method
log10ws	-7.13		Crippen Method
logp	6.815		Crippen Method
mcvol	296.400	ml/mol	McGowan Method
pc	1136.73	kPa	Joback Method
rinpol	2287.00		NIST Webbook
rinpol	2287.00		NIST Webbook
tb	761.95	K	Joback Method
tc	942.76	K	Joback Method
tf	409.62	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	859.08	J/mol×K	761.95	Joback Method
cpg	876.39	J/mol×K	792.08	Joback Method
cpg	892.79	J/mol×K	822.22	Joback Method
cpg	908.32	J/mol×K	852.35	Joback Method
cpg	922.99	J/mol×K	882.49	Joback Method
cpg	936.84	J/mol×K	912.62	Joback Method
cpg	949.89	J/mol×K	942.76	Joback Method
dvisc	0.0015155	Pa×s	409.62	Joback Method

dvisc	0.0006523	Pa×s	468.34	Joback Method
dvisc	0.0003388	Pa×s	527.06	Joback Method
dvisc	0.0002006	Pa×s	585.79	Joback Method
dvisc	0.0001307	Pa×s	644.51	Joback Method
dvisc	0.0000915	Pa×s	703.23	Joback Method
dvisc	0.0000677	Pa×s	761.95	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R248327&Units=SI

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