2,2-dichloroethyl hexadecanoate

Inchi: InChI=1S/C18H34Cl2O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18(21)22-16-17(19)20/h1
InchiKey: KHCNMQCCZLLSQF-UHFFFAOYSA-N
Formula: C18H34Cl2O2
SMILES: CCCCCCCCCCCCCCCC(=O)OCC(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	2301.00		NIST Webbook
rinpol	2301.00		NIST Webbook
rinpol	2301.00		NIST Webbook
rinpol	2293.00		NIST Webbook
rinpol	2293.00		NIST Webbook
ripol	2780.00		NIST Webbook
ripol	2780.00		NIST Webbook
ripol	2765.00		NIST Webbook
ripol	2792.00		NIST Webbook
ripol	2785.00		NIST Webbook
ripol	2781.00		NIST Webbook
ripol	2765.00		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

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=R30634&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume