2,2-dichloroethyl nonadecanoate

Inchi: InChI=1S/C21H40Cl2O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21(24)25-19-20
InchiKey: OJEQUJXADVZLKE-UHFFFAOYSA-N
Formula: C21H40Cl2O2
SMILES: CCCCCCCCCCCCCCCCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 395.45

Physical Properties

Property code	Value	Unit	Source
gf	-134.28	kJ/mol	Joback Method
hf	-758.33	kJ/mol	Joback Method
hfus	57.80	kJ/mol	Joback Method
hvap	79.88	kJ/mol	Joback Method
log10ws	-8.39		Crippen Method
logp	7.985		Crippen Method
mcvol	338.670	ml/mol	McGowan Method
pc	944.42	kPa	Joback Method
rinpol	2603.00		NIST Webbook
rinpol	2608.00		NIST Webbook
ripol	3087.00		NIST Webbook
ripol	3091.00		NIST Webbook
ripol	3096.00		NIST Webbook
ripol	3101.00		NIST Webbook
ripol	3096.00		NIST Webbook
tb	830.59	K	Joback Method
tc	1018.49	K	Joback Method
tf	443.43	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1039.05	J/mol×K	830.59	Joback Method
cpg	1057.60	J/mol×K	861.91	Joback Method
cpg	1075.10	J/mol×K	893.22	Joback Method

cpg	1091.58	J/mol×K	924.54	Joback Method
cpg	1107.08	J/mol×K	955.86	Joback Method
cpg	1121.64	J/mol×K	987.17	Joback Method
cpg	1135.29	J/mol×K	1018.49	Joback Method
dvisc	0.0010572	Pa×s	443.43	Joback Method
dvisc	0.0004430	Pa×s	507.96	Joback Method
dvisc	0.0002258	Pa×s	572.48	Joback Method
dvisc	0.0001319	Pa×s	637.01	Joback Method
dvisc	0.0000851	Pa×s	701.54	Joback Method
dvisc	0.0000591	Pa×s	766.06	Joback Method
dvisc	0.0000434	Pa×s	830.59	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=R30652&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