2,2-dichloroethyl dodecanoate

Inchi: InChI=1S/C14H26Cl2O2/c1-2-3-4-5-6-7-8-9-10-11-14(17)18-12-13(15)16/h13H,2-12H2,1
InchiKey: SLXXTAXPTODKMS-UHFFFAOYSA-N
Formula: C14H26Cl2O2
SMILES: CCCCCCCCCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 297.26

Physical Properties

Property code	Value	Unit	Source
gf	-193.22	kJ/mol	Joback Method
hf	-613.85	kJ/mol	Joback Method
hfus	39.67	kJ/mol	Joback Method
hvap	64.30	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	5.254		Crippen Method
mcvol	240.040	ml/mol	McGowan Method
pc	1499.99	kPa	Joback Method
rinpol	1880.00		NIST Webbook
rinpol	1891.00		NIST Webbook
rinpol	1884.00		NIST Webbook
rinpol	1899.00		NIST Webbook
rinpol	1893.00		NIST Webbook
ripol	2392.00		NIST Webbook
ripol	2363.00		NIST Webbook
ripol	2392.00		NIST Webbook
ripol	2378.00		NIST Webbook
ripol	2373.00		NIST Webbook
ripol	2354.00		NIST Webbook
ripol	2357.00		NIST Webbook
ripol	2348.00		NIST Webbook
ripol	2348.00		NIST Webbook
tb	670.43	K	Joback Method
tc	850.28	K	Joback Method
tf	364.54	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.04	J/mol×K	670.43	Joback Method
cpg	648.69	J/mol×K	700.41	Joback Method
cpg	663.57	J/mol×K	730.38	Joback Method
cpg	677.72	J/mol×K	760.36	Joback Method
cpg	691.13	J/mol×K	790.33	Joback Method
cpg	703.85	J/mol×K	820.31	Joback Method
cpg	715.87	J/mol×K	850.28	Joback Method
dvisc	0.0023096	Pa×s	364.54	Joback Method
dvisc	0.0010376	Pa×s	415.52	Joback Method
dvisc	0.0005552	Pa×s	466.50	Joback Method
dvisc	0.0003361	Pa×s	517.49	Joback Method
dvisc	0.0002226	Pa×s	568.47	Joback Method
dvisc	0.0001578	Pa×s	619.45	Joback Method
dvisc	0.0001178	Pa×s	670.43	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=R30595&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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