2,2-dichloroethyl tetradecanoate

Inchi: InChI=1S/C16H30Cl2O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-16(19)20-14-15(17)18/h15H,2-1
InchiKey: KRXOLTOZVXFYRG-UHFFFAOYSA-N
Formula: C16H30Cl2O2
SMILES: CCCCCCCCCCCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 325.31

Physical Properties

Property code	Value	Unit	Source
gf	-176.38	kJ/mol	Joback Method
hf	-655.13	kJ/mol	Joback Method
hfus	44.85	kJ/mol	Joback Method
hvap	68.75	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	6.034		Crippen Method
mcvol	268.220	ml/mol	McGowan Method
pc	1299.53	kPa	Joback Method
rinpol	2092.00		NIST Webbook
rinpol	2082.00		NIST Webbook
rinpol	2095.00		NIST Webbook
rinpol	2082.00		NIST Webbook
rinpol	2095.00		NIST Webbook
ripol	2573.00		NIST Webbook
ripol	2558.00		NIST Webbook
ripol	2573.00		NIST Webbook
ripol	2590.00		NIST Webbook
ripol	2581.00		NIST Webbook
ripol	2579.00		NIST Webbook
ripol	2560.00		NIST Webbook
ripol	2558.00		NIST Webbook
tb	716.19	K	Joback Method
tc	895.49	K	Joback Method
tf	387.08	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.82	J/mol×K	716.19	Joback Method
cpg	760.33	J/mol×K	746.07	Joback Method
cpg	776.01	J/mol×K	775.96	Joback Method
cpg	790.89	J/mol×K	805.84	Joback Method
cpg	804.98	J/mol×K	835.72	Joback Method
cpg	818.31	J/mol×K	865.61	Joback Method
cpg	830.90	J/mol×K	895.49	Joback Method
dvisc	0.0018889	Pa×s	387.08	Joback Method
dvisc	0.0008297	Pa×s	441.93	Joback Method
dvisc	0.0004370	Pa×s	496.78	Joback Method
dvisc	0.0002615	Pa×s	551.63	Joback Method
dvisc	0.0001717	Pa×s	606.49	Joback Method
dvisc	0.0001209	Pa×s	661.34	Joback Method
dvisc	0.0000898	Pa×s	716.19	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R30723&Units=SI
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

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