2,2-dichloroethyl pentadecanoate

Inchi: InChI=1S/C17H32Cl2O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17(20)21-15-16(18)19/h16H
InchiKey: OJAFDGARFLKHJC-UHFFFAOYSA-N
Formula: C17H32Cl2O2
SMILES: CCCCCCCCCCCCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 339.34

Physical Properties

Property code	Value	Unit	Source
gf	-167.96	kJ/mol	Joback Method
hf	-675.77	kJ/mol	Joback Method
hfus	47.44	kJ/mol	Joback Method
hvap	70.97	kJ/mol	Joback Method
log10ws	-6.71		Crippen Method
logp	6.425		Crippen Method
mcvol	282.310	ml/mol	McGowan Method
pc	1214.05	kPa	Joback Method
rinpol	2197.00		NIST Webbook
rinpol	2184.00		NIST Webbook
rinpol	2184.00		NIST Webbook
rinpol	2193.00		NIST Webbook
rinpol	2197.00		NIST Webbook
ripol	2692.00		NIST Webbook
ripol	2679.00		NIST Webbook
ripol	2680.00		NIST Webbook
ripol	2659.00		NIST Webbook
ripol	2679.00		NIST Webbook
ripol	2659.00		NIST Webbook
ripol	2663.00		NIST Webbook
ripol	2682.00		NIST Webbook
tb	739.07	K	Joback Method
tc	918.84	K	Joback Method
tf	398.35	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	800.93	J/mol×K	739.07	Joback Method
cpg	817.84	J/mol×K	769.03	Joback Method
cpg	833.89	J/mol×K	798.99	Joback Method
cpg	849.10	J/mol×K	828.95	Joback Method
cpg	863.49	J/mol×K	858.92	Joback Method
cpg	877.09	J/mol×K	888.88	Joback Method
cpg	889.92	J/mol×K	918.84	Joback Method
dvisc	0.0016957	Pa×s	398.35	Joback Method
dvisc	0.0007371	Pa×s	455.14	Joback Method
dvisc	0.0003855	Pa×s	511.92	Joback Method
dvisc	0.0002294	Pa×s	568.71	Joback Method
dvisc	0.0001501	Pa×s	625.50	Joback Method
dvisc	0.0001053	Pa×s	682.28	Joback Method
dvisc	0.0000781	Pa×s	739.07	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=R30698&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