2,2-dichloroethyl heptadecanoate

Inchi: InChI=1S/C19H36Cl2O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19(22)23-17-18(20)21
InchiKey: ZETLRULNQVZDBY-UHFFFAOYSA-N
Formula: C19H36Cl2O2
SMILES: CCCCCCCCCCCCCCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 367.39

Physical Properties

Property code	Value	Unit	Source
gf	-151.12	kJ/mol	Joback Method
hf	-717.05	kJ/mol	Joback Method
hfus	52.62	kJ/mol	Joback Method
hvap	75.43	kJ/mol	Joback Method
log10ws	-7.55		Crippen Method
logp	7.205		Crippen Method
mcvol	310.490	ml/mol	McGowan Method
pc	1066.57	kPa	Joback Method
rinpol	2395.00		NIST Webbook
rinpol	2405.00		NIST Webbook
rinpol	2402.00		NIST Webbook
rinpol	2395.00		NIST Webbook
rinpol	2405.00		NIST Webbook
ripol	2868.00		NIST Webbook
ripol	2895.00		NIST Webbook
ripol	2888.00		NIST Webbook
ripol	2868.00		NIST Webbook
ripol	2887.00		NIST Webbook
ripol	2884.00		NIST Webbook
tb	784.83	K	Joback Method
tc	967.30	K	Joback Method
tf	420.89	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.20	J/mol×K	784.83	Joback Method
cpg	997.54	J/mol×K	936.89	Joback Method
cpg	983.45	J/mol×K	906.48	Joback Method
cpg	968.50	J/mol×K	876.07	Joback Method
cpg	952.66	J/mol×K	845.65	Joback Method
cpg	935.90	J/mol×K	815.24	Joback Method
cpg	1010.80	J/mol×K	967.30	Joback Method
dvisc	0.0000585	Pa×s	784.83	Joback Method
dvisc	0.0000793	Pa×s	724.17	Joback Method
dvisc	0.0001136	Pa×s	663.52	Joback Method
dvisc	0.0001749	Pa×s	602.86	Joback Method
dvisc	0.0002968	Pa×s	542.20	Joback Method
dvisc	0.0005752	Pa×s	481.55	Joback Method
dvisc	0.0013490	Pa×s	420.89	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=R30616&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