2,2-dichloroethyl tridecanoate

Inchi: InChI=1S/C15H28Cl2O2/c1-2-3-4-5-6-7-8-9-10-11-12-15(18)19-13-14(16)17/h14H,2-13H
InchiKey: NDWBXUPQNOFSNY-UHFFFAOYSA-N
Formula: C15H28Cl2O2
SMILES: CCCCCCCCCCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 311.29

Physical Properties

Property code	Value	Unit	Source
gf	-184.80	kJ/mol	Joback Method
hf	-634.49	kJ/mol	Joback Method
hfus	42.26	kJ/mol	Joback Method
hvap	66.52	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	5.644		Crippen Method
mcvol	254.130	ml/mol	McGowan Method
pc	1394.37	kPa	Joback Method
rinpol	1981.00		NIST Webbook
rinpol	1992.00		NIST Webbook
rinpol	1998.00		NIST Webbook
rinpol	1986.00		NIST Webbook
rinpol	1981.00		NIST Webbook
rinpol	1993.00		NIST Webbook
rinpol	1993.00		NIST Webbook
ripol	2456.00		NIST Webbook
ripol	2457.00		NIST Webbook
ripol	2476.00		NIST Webbook
ripol	2479.00		NIST Webbook
ripol	2491.00		NIST Webbook
ripol	2467.00		NIST Webbook
ripol	2467.00		NIST Webbook
ripol	2456.00		NIST Webbook
tb	693.31	K	Joback Method
tc	872.65	K	Joback Method
tf	375.81	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	687.83	J/mol×K	693.31	Joback Method
cpg	760.55	J/mol×K	842.76	Joback Method
cpg	747.52	J/mol×K	812.87	Joback Method
cpg	733.75	J/mol×K	782.98	Joback Method
cpg	719.22	J/mol×K	753.09	Joback Method
cpg	703.92	J/mol×K	723.20	Joback Method
cpg	772.87	J/mol×K	872.65	Joback Method
dvisc	0.0001030	Pa×s	693.31	Joback Method
dvisc	0.0001383	Pa×s	640.39	Joback Method
dvisc	0.0001959	Pa×s	587.48	Joback Method
dvisc	0.0002970	Pa×s	534.56	Joback Method
dvisc	0.0004936	Pa×s	481.64	Joback Method
dvisc	0.0009300	Pa×s	428.73	Joback Method
dvisc	0.0020942	Pa×s	375.81	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R30737&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

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