2,2-dichloroethyl octadecanoate

Inchi: InChI=1S/C20H38Cl2O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20(23)24-18-19(21
InchiKey: RUPHJTBMXWPBGU-UHFFFAOYSA-N
Formula: C20H38Cl2O2
SMILES: CCCCCCCCCCCCCCCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 381.42

Physical Properties

Property code	Value	Unit	Source
gf	-142.70	kJ/mol	Joback Method
hf	-737.69	kJ/mol	Joback Method
hfus	55.21	kJ/mol	Joback Method
hvap	77.65	kJ/mol	Joback Method
log10ws	-7.97		Crippen Method
logp	7.595		Crippen Method
mcvol	324.580	ml/mol	McGowan Method
pc	1002.71	kPa	Joback Method
rinpol	2503.00		NIST Webbook
rinpol	2507.00		NIST Webbook
rinpol	2507.00		NIST Webbook
ripol	2985.00		NIST Webbook
ripol	2988.00		NIST Webbook
ripol	2999.00		NIST Webbook
ripol	2992.00		NIST Webbook
ripol	2985.00		NIST Webbook
tb	807.71	K	Joback Method
tc	992.53	K	Joback Method
tf	432.16	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	978.21	J/mol×K	807.71	Joback Method
cpg	996.33	J/mol×K	838.51	Joback Method

cpg	1013.45	J/mol×K	869.32	Joback Method
cpg	1029.61	J/mol×K	900.12	Joback Method
cpg	1044.83	J/mol×K	930.92	Joback Method
cpg	1059.15	J/mol×K	961.72	Joback Method
cpg	1072.61	J/mol×K	992.53	Joback Method
dvisc	0.0011963	Pa×s	432.16	Joback Method
dvisc	0.0005055	Pa×s	494.75	Joback Method
dvisc	0.0002592	Pa×s	557.34	Joback Method
dvisc	0.0001521	Pa×s	619.93	Joback Method
dvisc	0.0000984	Pa×s	682.53	Joback Method
dvisc	0.0000685	Pa×s	745.12	Joback Method
dvisc	0.0000505	Pa×s	807.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R30670&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

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