2,2-dichloroethyl eicosanoate

Inchi: InChI=1S/C22H42Cl2O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22(25)26-20
InchiKey: GQOAJQKJBXTXBR-UHFFFAOYSA-N
Formula: C22H42Cl2O2
SMILES: CCCCCCCCCCCCCCCCCCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 409.47

Physical Properties

Property code	Value	Unit	Source
gf	-125.86	kJ/mol	Joback Method
hf	-778.97	kJ/mol	Joback Method
hfus	60.39	kJ/mol	Joback Method
hvap	82.10	kJ/mol	Joback Method
log10ws	-8.81		Crippen Method
logp	8.375		Crippen Method
mcvol	352.760	ml/mol	McGowan Method
pc	891.07	kPa	Joback Method
rinpol	2708.00		NIST Webbook
rinpol	2704.00		NIST Webbook
rinpol	2708.00		NIST Webbook
rinpol	2704.00		NIST Webbook
ripol	3199.00		NIST Webbook
ripol	3199.00		NIST Webbook
ripol	3203.00		NIST Webbook
ripol	3194.00		NIST Webbook
ripol	3189.00		NIST Webbook
ripol	3189.00		NIST Webbook
tb	853.47	K	Joback Method
tc	1045.26	K	Joback Method
tf	454.70	K	Joback Method
vc	1.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	1100.65	J/mol×K	853.47	Joback Method
cpg	1119.66	J/mol×K	885.44	Joback Method
cpg	1137.56	J/mol×K	917.40	Joback Method
cpg	1154.38	J/mol×K	949.37	Joback Method
cpg	1170.17	J/mol×K	981.33	Joback Method
cpg	1184.97	J/mol×K	1013.30	Joback Method
cpg	1198.81	J/mol×K	1045.26	Joback Method
dvisc	0.0009313	Pa×s	454.70	Joback Method
dvisc	0.0003871	Pa×s	521.16	Joback Method
dvisc	0.0001962	Pa×s	587.62	Joback Method
dvisc	0.0001142	Pa×s	654.09	Joback Method
dvisc	0.0000734	Pa×s	720.55	Joback Method
dvisc	0.0000509	Pa×s	787.01	Joback Method
dvisc	0.0000373	Pa×s	853.47	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R30602&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