2-Chloroethyl palmitate

Other names: 2-Chloroethyl hexadecanoate
Hexadecanoic acid, 2-chloroethyl ester
NSC 406555
Inchi: InChI=1S/C18H35ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18(20)21-17-16-19/h2-17H
InchiKey: CPFFARIYTPCNJA-UHFFFAOYSA-N
Formula: C18H35ClO2
SMILES: CCCCCCCCCCCCCCCC(=O)OCCCl
Mol. weight [g/mol]: 318.92
CAS: 929-16-8

Physical Properties

Property code	Value	Unit	Source
gf	-145.17	kJ/mol	Joback Method
hf	-675.39	kJ/mol	Joback Method
hfus	49.36	kJ/mol	Joback Method
hvap	69.20	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	6.250		Crippen Method
mcvol	284.160	ml/mol	McGowan Method
pc	1159.29	kPa	Joback Method
rinpol	2202.00		NIST Webbook
rinpol	2207.00		NIST Webbook
rinpol	2207.00		NIST Webbook
rinpol	2196.00		NIST Webbook
rinpol	2196.00		NIST Webbook
ripol	2672.00		NIST Webbook
ripol	2690.00		NIST Webbook
ripol	2701.00		NIST Webbook
ripol	2692.00		NIST Webbook
ripol	2691.00		NIST Webbook
ripol	2675.00		NIST Webbook
tb	724.96	K	Joback Method
tc	898.71	K	Joback Method
tf	394.70	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.31	J/mol×K	724.96	Joback Method
cpg	906.90	J/mol×K	869.75	Joback Method
cpg	892.21	J/mol×K	840.79	Joback Method
cpg	876.73	J/mol×K	811.84	Joback Method
cpg	860.43	J/mol×K	782.88	Joback Method
cpg	843.30	J/mol×K	753.92	Joback Method
cpg	920.82	J/mol×K	898.71	Joback Method
dvisc	0.0000844	Pa×s	724.96	Joback Method
dvisc	0.0001127	Pa×s	669.92	Joback Method
dvisc	0.0001583	Pa×s	614.87	Joback Method
dvisc	0.0002378	Pa×s	559.83	Joback Method
dvisc	0.0003904	Pa×s	504.79	Joback Method
dvisc	0.0007235	Pa×s	449.74	Joback Method
dvisc	0.0015927	Pa×s	394.70	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C929168&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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