

2-chloroethyl octadecanoate

Inchi: InChI=1S/C20H39ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20(22)23-19-18-21
InchiKey: QLBIYHGOHHPBCC-UHFFFAOYSA-N
Formula: C20H39ClO2
SMILES: CCCCCCCCCCCCCCCCCC(=O)OCCCl
Mol. weight [g/mol]: 346.98

Physical Properties

Property code	Value	Unit	Source
gf	-128.33	kJ/mol	Joback Method
hf	-716.67	kJ/mol	Joback Method
hfus	54.54	kJ/mol	Joback Method
hvap	73.66	kJ/mol	Joback Method
log10ws	-7.21		Crippen Method
logp	7.030		Crippen Method
mcvol	312.340	ml/mol	McGowan Method
pc	1021.38	kPa	Joback Method
ripol	2403.00		NIST Webbook
ripol	2409.00		NIST Webbook
ripol	2411.00		NIST Webbook
ripol	2881.00		NIST Webbook
ripol	2895.00		NIST Webbook
ripol	2897.00		NIST Webbook
ripol	2904.00		NIST Webbook
ripol	2900.00		NIST Webbook
tb	770.72	K	Joback Method
tc	948.17	K	Joback Method
tf	417.24	K	Joback Method
vc	1.228	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	944.23	J/molxK	770.72	Joback Method
cpg	1029.30	J/molxK	918.60	Joback Method

cpg	1014.07	J/mol×K	889.02	Joback Method
cpg	997.98	J/mol×K	859.45	Joback Method
cpg	980.99	J/mol×K	829.87	Joback Method
cpg	963.08	J/mol×K	800.30	Joback Method
cpg	1043.68	J/mol×K	948.17	Joback Method
dvisc	0.0000640	Paxs	770.72	Joback Method
dvisc	0.0000858	Paxs	711.81	Joback Method
dvisc	0.0001213	Paxs	652.89	Joback Method
dvisc	0.0001837	Paxs	593.98	Joback Method
dvisc	0.0003049	Paxs	535.07	Joback Method
dvisc	0.0005737	Paxs	476.15	Joback Method
dvisc	0.0012902	Paxs	417.24	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=R30844&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

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