

4-Chlorobutyric acid, octadecyl ester

Other names:	Octadecyl 4-chlorobutanoate
Inchi:	InChI=1S/C22H43ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-25-22(24)19-18
InchiKey:	PENLVWCLIVDARD-UHFFFAOYSA-N
Formula:	C22H43ClO2
SMILES:	CCCCCCCCCCCCCCCCCCCCOC(=O)CCCCl
Mol. weight [g/mol]:	375.03

Physical Properties

Property code	Value	Unit	Source
gf	-111.49	kJ/mol	Joback Method
hf	-757.95	kJ/mol	Joback Method
hfus	59.72	kJ/mol	Joback Method
hvap	78.11	kJ/mol	Joback Method
log10ws	-8.05		Crippen Method
logp	7.810		Crippen Method
mcvol	340.520	ml/mol	McGowan Method
pc	906.70	kPa	Joback Method
rinpol	2608.00		NIST Webbook
tb	816.48	K	Joback Method
tc	1000.37	K	Joback Method
tf	439.78	K	Joback Method
vc	1.341	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1066.74	J/molxK	816.48	Joback Method
cpg	1086.54	J/molxK	847.13	Joback Method
cpg	1105.29	J/molxK	877.78	Joback Method
cpg	1123.00	J/molxK	908.43	Joback Method
cpg	1139.72	J/molxK	939.07	Joback Method
cpg	1155.47	J/molxK	969.72	Joback Method
cpg	1170.29	J/molxK	1000.37	Joback Method
dvisc	0.0010274	Paxs	439.78	Joback Method

dvisc	0.0004480	Paxs	502.56	Joback Method
dvisc	0.0002349	Paxs	565.35	Joback Method
dvisc	0.0001402	Paxs	628.13	Joback Method
dvisc	0.0000918	Paxs	690.91	Joback Method
dvisc	0.0000646	Paxs	753.70	Joback Method
dvisc	0.0000479	Paxs	816.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U340235&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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