

Hexadecyl 3-chlorobutanoate

Other names:	Butanoic acid, 3-chloro, hexadecyl ester
Inchi:	InChI=1S/C20H39ClO2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-23-20(22)18-19(2)21
InchiKey:	UGGCAGSELNTZDI-UHFFFAOYSA-N
Formula:	C20H39ClO2
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CC(C)Cl
Mol. weight [g/mol]:	346.98

Physical Properties

Property code	Value	Unit	Source
gf	-130.77	kJ/mol	Joback Method
hf	-721.95	kJ/mol	Joback Method
hfus	51.02	kJ/mol	Joback Method
hvap	73.27	kJ/mol	Joback Method
log10ws	-7.32		Crippen Method
logp	7.028		Crippen Method
mcvol	312.340	ml/mol	McGowan Method
pc	1026.63	kPa	Joback Method
rinpol	2333.00		NIST Webbook
rinpol	2333.00		NIST Webbook
rinpol	2342.00		NIST Webbook
rinpol	2338.00		NIST Webbook
tb	770.28	K	Joback Method
tc	948.76	K	Joback Method
tf	402.24	K	Joback Method
vc	1.222	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	944.69	J/molxK	770.28	Joback Method
cpg	963.67	J/molxK	800.03	Joback Method
cpg	981.68	J/molxK	829.77	Joback Method
cpg	998.75	J/molxK	859.52	Joback Method
cpg	1014.91	J/molxK	889.27	Joback Method

cpg	1030.18	J/molxK	919.02	Joback Method
cpg	1044.59	J/molxK	948.76	Joback Method
dvisc	0.0015827	Paxs	402.24	Joback Method
dvisc	0.0006361	Paxs	463.58	Joback Method
dvisc	0.0003163	Paxs	524.92	Joback Method
dvisc	0.0001821	Paxs	586.26	Joback Method
dvisc	0.0001164	Paxs	647.60	Joback Method
dvisc	0.0000804	Paxs	708.94	Joback Method
dvisc	0.0000589	Paxs	770.28	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=R28241&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
hvac:	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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