

6-Chlorohexanoic acid, 3-methylbutyl ester

Inchi:	InChI=1S/C11H21ClO2/c1-10(2)7-9-14-11(13)6-4-3-5-8-12/h10H,3-9H2,1-2H3
InchiKey:	NDBJAENHHLJARY-UHFFFAOYSA-N
Formula:	C11H21ClO2
SMILES:	CC(C)CCOC(=O)CCCCCCl
Mol. weight [g/mol]:	220.74

Physical Properties

Property code	Value	Unit	Source
gf	-206.55	kJ/mol	Joback Method
hf	-536.19	kJ/mol	Joback Method
hfus	27.71	kJ/mol	Joback Method
hvap	53.23	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	3.375		Crippen Method
mcvol	185.530	ml/mol	McGowan Method
pc	1963.07	kPa	Joback Method
rinpola	1546.00		NIST Webbook
tb	564.36	K	Joback Method
tc	743.50	K	Joback Method
tf	300.81	K	Joback Method
vc	0.719	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.93	J/molxK	564.36	Joback Method
cpg	461.63	J/molxK	594.22	Joback Method
cpg	475.70	J/molxK	624.07	Joback Method
cpg	489.15	J/molxK	653.93	Joback Method
cpg	501.98	J/molxK	683.78	Joback Method
cpg	514.22	J/molxK	713.64	Joback Method
cpg	525.87	J/molxK	743.50	Joback Method
dvisc	0.0036823	Paxs	300.81	Joback Method
dvisc	0.0016303	Paxs	344.74	Joback Method

dvisc	0.0008677	Paxs	388.66	Joback Method
dvisc	0.0005249	Paxs	432.59	Joback Method
dvisc	0.0003484	Paxs	476.51	Joback Method
dvisc	0.0002478	Paxs	520.44	Joback Method
dvisc	0.0001859	Paxs	564.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354726&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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