

Ketone, chloromethyl hexahydro-6-hydroxyidan-1-yl

Inchi:	InChI=1S/C11H17ClO2/c12-6-11(14)9-4-2-7-1-3-8(13)5-10(7)9/h7-10,13H,1-6H2
InchiKey:	UGZFMUIJAVIJS-UHFFFAOYSA-N
Formula:	C11H17ClO2
SMILES:	O=C(CCl)C1CCC2CCC(O)CC21
Mol. weight [g/mol]:	216.70
CAS:	116373-84-3

Physical Properties

Property code	Value	Unit	Source
gf	-166.15	kJ/mol	Joback Method
hf	-464.48	kJ/mol	Joback Method
hfus	26.24	kJ/mol	Joback Method
hvap	67.61	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.982		Crippen Method
mcvol	163.810	ml/mol	McGowan Method
pc	2808.38	kPa	Joback Method
tb	651.51	K	Joback Method
tc	859.35	K	Joback Method
tf	371.24	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.41	J/molxK	651.51	Joback Method
cpg	477.33	J/molxK	686.15	Joback Method
cpg	492.24	J/molxK	720.79	Joback Method
cpg	506.18	J/molxK	755.43	Joback Method
cpg	519.19	J/molxK	790.07	Joback Method
cpg	531.33	J/molxK	824.71	Joback Method
cpg	542.63	J/molxK	859.35	Joback Method
dvisc	0.0053230	Paxs	371.24	Joback Method
dvisc	0.0024361	Paxs	417.95	Joback Method

dvisc	0.0013046	Paxs	464.66	Joback Method
dvisc	0.0007831	Paxs	511.38	Joback Method
dvisc	0.0005120	Paxs	558.09	Joback Method
dvisc	0.0003574	Paxs	604.80	Joback Method
dvisc	0.0002627	Paxs	651.51	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116373843&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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