

5-Chlorovaleric acid, hexyl ester

Inchi:	InChI=1S/C11H21ClO2/c1-2-3-4-7-10-14-11(13)8-5-6-9-12/h2-10H2,1H3
InchiKey:	ZFVGXJLTIIOW-UHFFFAOYSA-N
Formula:	C11H21ClO2
SMILES:	CCCCCOC(=O)CCCCCl
Mol. weight [g/mol]:	220.74
CAS:	2323-66-2

Physical Properties

Property code	Value	Unit	Source
gf	-204.11	kJ/mol	Joback Method
hf	-530.91	kJ/mol	Joback Method
hfus	31.23	kJ/mol	Joback Method
hvap	53.62	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.519		Crippen Method
mvol	185.530	ml/mol	McGowan Method
pc	1949.23	kPa	Joback Method
rinpol	1545.40		NIST Webbook
tb	564.80	K	Joback Method
tc	740.70	K	Joback Method
tf	315.81	K	Joback Method
vc	0.725	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.60	J/molxK	564.80	Joback Method
cpg	460.98	J/molxK	594.12	Joback Method
cpg	474.76	J/molxK	623.43	Joback Method
cpg	487.95	J/molxK	652.75	Joback Method
cpg	500.56	J/molxK	682.07	Joback Method
cpg	512.59	J/molxK	711.39	Joback Method
cpg	524.06	J/molxK	740.70	Joback Method
dvisc	0.0027568	Paxs	315.81	Joback Method

dvisc	0.0013779	Paxs	357.31	Joback Method
dvisc	0.0007956	Paxs	398.81	Joback Method
dvisc	0.0005095	Paxs	440.30	Joback Method
dvisc	0.0003523	Paxs	481.80	Joback Method
dvisc	0.0002583	Paxs	523.30	Joback Method
dvisc	0.0001982	Paxs	564.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2323662&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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