

5-Chlorovaleric acid, decyl ester

Inchi:	InChI=1S/C15H29ClO2/c1-2-3-4-5-6-7-8-11-14-18-15(17)12-9-10-13-16/h2-14H2,1H3
InchiKey:	GDDOSYXFHTVPTR-UHFFFAOYSA-N
Formula:	C15H29ClO2
SMILES:	CCCCCCCCCOC(=O)CCCCCl
Mol. weight [g/mol]:	276.84
CAS:	52893-19-3

Physical Properties

Property code	Value	Unit	Source
gf	-170.43	kJ/mol	Joback Method
hf	-613.47	kJ/mol	Joback Method
hfus	41.59	kJ/mol	Joback Method
hvap	62.52	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	5.079		Crippen Method
mcvol	241.890	ml/mol	McGowan Method
pc	1425.07	kPa	Joback Method
rinpol	1982.00		NIST Webbook
rinpol	1982.00		NIST Webbook
tb	656.32	K	Joback Method
tc	828.65	K	Joback Method
tf	360.89	K	Joback Method
vc	0.949	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.00	J/mol×K	656.32	Joback Method
cpg	671.67	J/mol×K	685.04	Joback Method
cpg	687.59	J/mol×K	713.76	Joback Method
cpg	702.78	J/mol×K	742.49	Joback Method
cpg	717.25	J/mol×K	771.21	Joback Method
cpg	731.03	J/mol×K	799.93	Joback Method
cpg	744.13	J/mol×K	828.65	Joback Method

dvisc	0.0021007	Paxs	360.89	Joback Method
dvisc	0.0009897	Paxs	410.13	Joback Method
dvisc	0.0005479	Paxs	459.37	Joback Method
dvisc	0.0003401	Paxs	508.60	Joback Method
dvisc	0.0002297	Paxs	557.84	Joback Method
dvisc	0.0001653	Paxs	607.08	Joback Method
dvisc	0.0001250	Paxs	656.32	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=C52893193&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
mvol:	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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