

5-Chlorovaleric acid, tridecyl ester

Inchi:	InChI=1S/C18H35ClO2/c1-2-3-4-5-6-7-8-9-10-11-14-17-21-18(20)15-12-13-16-19/h2-17
InchiKey:	QUAVOGDQRCBTGN-UHFFFAOYSA-N
Formula:	C18H35ClO2
SMILES:	CCCCCCCCCCCCOC(=O)CCCCCl
Mol. weight [g/mol]:	318.92

Physical Properties

Property code	Value	Unit	Source
gf	-145.17	kJ/mol	Joback Method
hf	-675.39	kJ/mol	Joback Method
hfus	49.36	kJ/mol	Joback Method
hvap	69.20	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	6.250		Crippen Method
mvol	284.160	ml/mol	McGowan Method
pc	1159.29	kPa	Joback Method
rinpol	2249.10		NIST Webbook
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tb	724.96	K	Joback Method
tc	898.71	K	Joback Method
tf	394.70	K	Joback Method
vc	1.117	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.31	J/molxK	724.96	Joback Method
cpg	906.90	J/molxK	869.75	Joback Method
cpg	892.21	J/molxK	840.79	Joback Method
cpg	876.73	J/molxK	811.84	Joback Method
cpg	860.43	J/molxK	782.88	Joback Method
cpg	843.30	J/molxK	753.92	Joback Method
cpg	920.82	J/molxK	898.71	Joback Method
dvisc	0.0000844	Paxs	724.96	Joback Method

dvisc	0.0001127	Paxs	669.92	Joback Method
dvisc	0.0001583	Paxs	614.87	Joback Method
dvisc	0.0002378	Paxs	559.83	Joback Method
dvisc	0.0003904	Paxs	504.79	Joback Method
dvisc	0.0007235	Paxs	449.74	Joback Method
dvisc	0.0015927	Paxs	394.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292314&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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