

5-Chlorovaleric acid, undecyl ester

Inchi:	InChI=1S/C16H31ClO2/c1-2-3-4-5-6-7-8-9-12-15-19-16(18)13-10-11-14-17/h2-15H2,1H3
InchiKey:	MZLDFDLDFGBNEV-UHFFFAOYSA-N
Formula:	C16H31ClO2
SMILES:	CCCCCCCCCCCCOC(=O)CCCCCI
Mol. weight [g/mol]:	290.87
CAS:	52893-20-6

Physical Properties

Property code	Value	Unit	Source
gf	-162.01	kJ/mol	Joback Method
hf	-634.11	kJ/mol	Joback Method
hfus	44.18	kJ/mol	Joback Method
hvap	64.75	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	5.470		Crippen Method
mcvol	255.980	ml/mol	McGowan Method
pc	1327.14	kPa	Joback Method
rinpol	2064.10		NIST Webbook
tb	679.20	K	Joback Method
tc	851.53	K	Joback Method
tf	372.16	K	Joback Method
vc	1.004	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.59	J/molxK	679.20	Joback Method
cpg	727.71	J/molxK	707.92	Joback Method
cpg	744.05	J/molxK	736.64	Joback Method
cpg	759.63	J/molxK	765.36	Joback Method
cpg	774.47	J/molxK	794.09	Joback Method
cpg	788.57	J/molxK	822.81	Joback Method
cpg	801.97	J/molxK	851.53	Joback Method
dvisc	0.0019268	Paxs	372.16	Joback Method

dvisc	0.0008962	Paxs	423.33	Joback Method
dvisc	0.0004917	Paxs	474.51	Joback Method
dvisc	0.0003032	Paxs	525.68	Joback Method
dvisc	0.0002037	Paxs	576.85	Joback Method
dvisc	0.0001460	Paxs	628.03	Joback Method
dvisc	0.0001101	Paxs	679.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52893206&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

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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