

5-Chlorovaleric acid, tetradecyl ester

Inchi:	InChI=1S/C19H37ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-15-18-22-19(21)16-13-14-17-20/h2-
InchiKey:	RUNXJNORIBCNLQ-UHFFFAOYSA-N
Formula:	C19H37ClO2
SMILES:	CCCCCCCCCCCCCOC(=O)CCCCCl
Mol. weight [g/mol]:	332.95

Physical Properties

Property code	Value	Unit	Source
gf	-136.75	kJ/mol	Joback Method
hf	-696.03	kJ/mol	Joback Method
hfus	51.95	kJ/mol	Joback Method
hvap	71.43	kJ/mol	Joback Method
log10ws	-6.79		Crippen Method
logp	6.640		Crippen Method
mcvol	298.250	ml/mol	McGowan Method
pc	1087.06	kPa	Joback Method
rinpol	2361.20		NIST Webbook
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tb	747.84	K	Joback Method
tc	923.13	K	Joback Method
tf	405.97	K	Joback Method
vc	1.173	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.28	J/mol×K	747.84	Joback Method
cpg	967.61	J/mol×K	893.91	Joback Method
cpg	952.65	J/mol×K	864.70	Joback Method
cpg	936.86	J/mol×K	835.48	Joback Method
cpg	920.22	J/mol×K	806.27	Joback Method
cpg	902.70	J/mol×K	777.05	Joback Method
cpg	981.77	J/mol×K	923.13	Joback Method
dvisc	0.0000736	Paxs	747.84	Joback Method

dvisc	0.0000984	Paxs	690.86	Joback Method
dvisc	0.0001388	Paxs	633.88	Joback Method
dvisc	0.0002094	Paxs	576.90	Joback Method
dvisc	0.0003456	Paxs	519.93	Joback Method
dvisc	0.0006456	Paxs	462.95	Joback Method
dvisc	0.0014368	Paxs	405.97	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=U292315&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
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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