

5-Chlorovaleric acid, tridec-2-ynyl ester

Inchi: InChI=1S/C18H31ClO2/c1-2-3-4-5-6-7-8-9-10-11-14-17-21-18(20)15-12-13-16-19/h2-10,
InchiKey: IWBWGAAOVXOGLS-UHFFFAOYSA-N
Formula: C18H31ClO2
SMILES: CCCCCCCCCC#CCOC(=O)CCCCCl
Mol. weight [g/mol]: 314.89

Physical Properties

Property code	Value	Unit	Source
gf	57.63	kJ/mol	Joback Method
hf	-403.09	kJ/mol	Joback Method
hfus	52.48	kJ/mol	Joback Method
hvap	71.36	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.473		Crippen Method
mvol	275.560	ml/mol	McGowan Method
pc	1296.73	kPa	Joback Method
rinpol	2284.70		NIST Webbook
rinpol	2284.70		NIST Webbook
tb	733.96	K	Joback Method
tc	918.92	K	Joback Method
tf	500.80	K	Joback Method
vc	1.079	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.93	J/mol×K	733.96	Joback Method
cpg	797.31	J/mol×K	764.79	Joback Method
cpg	813.81	J/mol×K	795.61	Joback Method
cpg	829.46	J/mol×K	826.44	Joback Method
cpg	844.27	J/mol×K	857.27	Joback Method
cpg	858.28	J/mol×K	888.10	Joback Method
cpg	871.49	J/mol×K	918.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292482&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
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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