5-Chlorovaleric acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C16H25ClO2/c1-5-8-14(4)15(11-10-13(2)3)19-16(18)9-6-7-12-17/h14-15H,2,5-

InchiKey: QPMAFXVSIZPLAK-UHFFFAOYSA-N

Formula: C16H25ClO2

SMILES: C=C(C)C#CC(OC(=O)CCCCCl)C(C)CCC

Mol. weight [g/mol]: 284.82

Physical Properties

Property code	Value	Unit	Source
gf	115.20	kJ/mol	Joback Method
hf	-256.73	kJ/mol	Joback Method
hfus	37.67	kJ/mol	Joback Method
hvap	65.54	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.323		Crippen Method
mcvol	243.080	ml/mol	McGowan Method
pc	1572.21	kPa	Joback Method
rinpol	1825.40		NIST Webbook
tb	683.88	K	Joback Method
tc	881.15	K	Joback Method
tf	432.54	K	Joback Method
vc	0.936	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.26	J/mol×K	683.88	Joback Method
cpg	661.11	J/mol×K	716.76	Joback Method
cpg	677.05	J/mol×K	749.64	Joback Method
cpg	692.13	J/mol×K	782.51	Joback Method
cpg	706.35	J/mol×K	815.39	Joback Method
cpg	719.76	J/mol×K	848.27	Joback Method
cpg	732.37	J/mol×K	881.15	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U292480&Units=SI

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
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