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]: 284.83

Physical Properties

Property code	Value	Unit	Source
hfus	37.67	kJ/mol	Joback Method
logp	4.323		Crippen Method
mcvol	243.080	ml/mol	McGowan Method
rinpol	1825.40		NIST Webbook

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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U292480&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices