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

Inchi: InChI=1S/C16H25BrO2/c1-5-8-14(4)15(11-10-13(2)3)19-16(18)9-6-7-12-17/h14-15H,2,5-

InchiKey: NSQUUHNKUHSLAD-UHFFFAOYSA-N

Formula: C16H25BrO2

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

Mol. weight [g/mol]: 329.27

Physical Properties

Property code	Value	Unit	Source
gf	141.45	kJ/mol	Joback Method
hf	-214.66	kJ/mol	Joback Method
hfus	38.75	kJ/mol	Joback Method
hvap	67.59	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.479		Crippen Method
mcvol	248.340	ml/mol	McGowan Method
pc	1713.19	kPa	Joback Method
rinpol	1914.00		NIST Webbook
rinpol	1914.00		NIST Webbook
tb	712.61	K	Joback Method
tc	916.84	K	Joback Method
tf	462.42	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.89	J/mol×K	712.61	Joback Method
cpg	676.40	J/mol×K	746.65	Joback Method
cpg	691.98	J/mol×K	780.69	Joback Method
cpg	706.68	J/mol×K	814.73	Joback Method
cpg	720.51	J/mol×K	848.76	Joback Method
cpg	733.53	J/mol×K	882.80	Joback Method
cpg	745.76	J/mol×K	916.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292569&Units=SI
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

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