5-Bromovaleric acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C14H23BrO2/c1-4-5-8-13(11-12(2)3)17-14(16)9-6-7-10-15/h12-13H,4,6-7,9-11

InchiKey: YQUNASOLAFZHPP-UHFFFAOYSA-N

Formula: C14H23BrO2

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

Mol. weight [g/mol]: 303.24

Physical Properties

Property code	Value	Unit	Source
gf	45.32	kJ/mol	Joback Method
hf	-289.02	kJ/mol	Joback Method
hfus	36.16	kJ/mol	Joback Method
hvap	63.72	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	3.923		Crippen Method
mcvol	224.460	ml/mol	McGowan Method
pc	1938.95	kPa	Joback Method
rinpol	1785.80		NIST Webbook
rinpol	1785.80		NIST Webbook
tb	670.29	K	Joback Method
tc	873.27	K	Joback Method
tf	455.60	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.90	J/mol×K	670.29	Joback Method
cpg	591.92	J/mol×K	704.12	Joback Method
cpg	607.08	J/mol×K	737.95	Joback Method
cpg	621.42	J/mol×K	771.78	Joback Method
cpg	634.94	J/mol×K	805.61	Joback Method
cpg	647.67	J/mol×K	839.44	Joback Method
cpg	659.65	J/mol×K	873.27	Joback Method

Sources

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=U292567&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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