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

Inchi: InChI=1S/C16H19BrO2/c1-4-5-6-15(11-12(2)3)19-16(18)13-7-9-14(17)10-8-13/h7-10,12,

InchiKey: KOBPOANEYWMGMK-UHFFFAOYSA-N

Formula: C16H19BrO2

SMILES: CCC#CC(CC(C)C)OC(=O)c1ccc(Br)cc1

Mol. weight [g/mol]: 323.23

Physical Properties

Property code	Value	Unit	Source
gf	164.94	kJ/mol	Joback Method
hf	-105.24	kJ/mol	Joback Method
hfus	35.00	kJ/mol	Joback Method
hvap	71.12	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	4.434		Crippen Method
mcvol	228.880	ml/mol	McGowan Method
pc	2169.38	kPa	Joback Method
rinpol	1967.00		NIST Webbook
rinpol	1967.00		NIST Webbook
tb	747.71	K	Joback Method
tc	982.45	K	Joback Method
tf	517.08	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.87	J/mol×K	747.71	Joback Method
cpg	613.43	J/mol×K	786.83	Joback Method
cpg	627.86	J/mol×K	825.96	Joback Method
cpg	641.23	J/mol×K	865.08	Joback Method
cpg	653.57	J/mol×K	904.21	Joback Method
cpg	664.94	J/mol×K	943.33	Joback Method
cpg	675.37	J/mol×K	982.45	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=U299248&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

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