4-Bromobenzoic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

Inchi: InChI=1S/C17H19BrO2/c1-12(2)5-10-16(11-13(3)4)20-17(19)14-6-8-15(18)9-7-14/h6-9,1

InchiKey: WAFMFZCHHZKUSJ-UHFFFAOYSA-N

Formula: C17H19BrO2

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

Mol. weight [g/mol]: 335.24

Physical Properties

Property code	Value	Unit	Source
gf	252.65	kJ/mol	Joback Method
hf	-10.24	kJ/mol	Joback Method
hfus	35.00	kJ/mol	Joback Method
hvap	72.75	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	4.600		Crippen Method
mcvol	238.670	ml/mol	McGowan Method
pc	2073.65	kPa	Joback Method
rinpol	2019.00		NIST Webbook
tb	767.15	K	Joback Method
tc	1005.46	K	Joback Method
tf	512.63	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.81	J/mol×K	767.15	Joback Method
cpg	642.31	J/mol×K	806.87	Joback Method
cpg	656.68	J/mol×K	846.59	Joback Method
cpg	669.97	J/mol×K	886.31	Joback Method
cpg	682.24	J/mol×K	926.02	Joback Method
cpg	693.54	J/mol×K	965.74	Joback Method
cpg	703.95	J/mol×K	1005.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299249&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