

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

Inchi:	InChI=1S/C17H19BrO2/c1-12(2)9-10-14(11-13(3)4)20-17(19)15-7-5-6-8-16(15)18/h5-8,1
InchiKey:	RTMJWOJEHVYKIA-UHFFFAOYSA-N
Formula:	C17H19BrO2
SMILES:	<chem>C=C(C)C#CC(CC(C)C)OC(=O)c1ccccc1Br</chem>
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	2000.00		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/molxK	767.15	Joback Method
cpg	642.31	J/molxK	806.87	Joback Method
cpg	656.68	J/molxK	846.59	Joback Method
cpg	669.97	J/molxK	886.31	Joback Method
cpg	682.24	J/molxK	926.02	Joback Method
cpg	693.54	J/molxK	965.74	Joback Method
cpg	703.95	J/molxK	1005.46	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299397&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

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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