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

Inchi: InChI=1S/C18H21BrO2/c1-5-7-14(4)17(11-10-13(2)3)21-18(20)15-8-6-9-16(19)12-15/h6,

InchiKey: XFEWWWKVYNRMDB-UHFFFAOYSA-N

Formula: C18H21BrO2

SMILES: C=C(C)C#CC(OC(=O)c1cccc(Br)c1)C(C)CCC

Mol. weight [g/mol]: 349.26

Physical Properties

Property code	Value	Unit	Source
gf	261.07	kJ/mol	Joback Method
hf	-30.88	kJ/mol	Joback Method
hfus	37.59	kJ/mol	Joback Method
hvap	74.98	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	4.990		Crippen Method
mcvol	252.760	ml/mol	McGowan Method
pc	1903.58	kPa	Joback Method
rinpol	2080.00		NIST Webbook
tb	790.03	K	Joback Method
tc	1024.16	K	Joback Method
tf	523.90	K	Joback Method
vc	0.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.94	J/mol×K	790.03	Joback Method
cpg	697.71	J/mol×K	829.05	Joback Method
cpg	712.35	J/mol×K	868.07	Joback Method
cpg	725.90	J/mol×K	907.09	Joback Method
cpg	738.43	J/mol×K	946.12	Joback Method
cpg	750.00	J/mol×K	985.14	Joback Method
cpg	760.67	J/mol×K	1024.16	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=U299146&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