4-Bromobenzoic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C13H13BrO2/c1-3-5-12(4-2)16-13(15)10-6-8-11(14)9-7-10/h6-9,12H,4H2,1-2H
InchiKey: JJVRBDULJATJQH-UHFFFAOYSA-N
Formula: C13H13BrO2
SMILES: CC#CC(CC)OC(=O)c1ccc(Br)cc1
Mol. weight [g/mol]: 281.14

Physical Properties

Property code	Value	Unit	Source
gf	142.12	kJ/mol	Joback Method
hf	-38.04	kJ/mol	Joback Method
hfus	30.75	kJ/mol	Joback Method
hvap	64.83	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.408		Crippen Method
mcvol	186.610	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
rinpol	1756.00		NIST Webbook
rinpol	1756.00		NIST Webbook
tb	679.51	K	Joback Method
tc	924.13	K	Joback Method
tf	498.27	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.47	J/mol×K	679.51	Joback Method
cpg	454.32	J/mol×K	720.28	Joback Method
cpg	467.17	J/mol×K	761.05	Joback Method
cpg	479.06	J/mol×K	801.82	Joback Method
cpg	490.04	J/mol×K	842.59	Joback Method
cpg	500.13	J/mol×K	883.36	Joback Method
cpg	509.37	J/mol×K	924.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299246&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
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