Benzeneacetic acid, 4-nitro-, but-3-yn-2-yl ester

Inchi: InChI=1S/C12H11NO4/c1-3-9(2)17-12(14)8-10-4-6-11(7-5-10)13(15)16/h1,4-7,9H,8H2,2

InchiKey: AWQCWUSSUFXPMK-UHFFFAOYSA-N

Formula: C12H11NO4

SMILES: C#CC(C)OC(=O)Cc1ccc([N+](=O)[O-])cc1

Mol. weight [g/mol]: 233.22

Physical Properties

Property code	Value	Unit	Source
gf	175.20	kJ/mol	Joback Method
hf	-34.89	kJ/mol	Joback Method
hfus	34.09	kJ/mol	Joback Method
hvap	70.46	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	1.702		Crippen Method
mcvol	172.440	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	1827.00		NIST Webbook
rinpol	1827.00		NIST Webbook
tb	723.43	K	Joback Method
tc	971.42	K	Joback Method
tf	511.68	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.44	J/mol×K	723.43	Joback Method
cpg	461.70	J/mol×K	764.76	Joback Method
cpg	472.94	J/mol×K	806.09	Joback Method
cpg	483.22	J/mol×K	847.42	Joback Method
cpg	492.56	J/mol×K	888.76	Joback Method
cpg	501.03	J/mol×K	930.09	Joback Method
cpg	508.65	J/mol×K	971.42	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=U406976&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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