4-Nitrobenzoic acid, but-3-yn-2-yl ester

Inchi: InChI=1S/C11H9NO4/c1-3-8(2)16-11(13)9-4-6-10(7-5-9)12(14)15/h1,4-8H,2H3
InchiKey: PLOONFHELCAORZ-UHFFFAOYSA-N
Formula: C11H9NO4
SMILES: C#CC(C)OC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 219.19

Physical Properties

Property code	Value	Unit	Source
gf	166.78	kJ/mol	Joback Method
hf	-14.25	kJ/mol	Joback Method
hfus	31.50	kJ/mol	Joback Method
hvap	68.23	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	1.773		Crippen Method
mcvol	158.350	ml/mol	McGowan Method
pc	3287.81	kPa	Joback Method
rinpol	1600.00		NIST Webbook
rinpol	1600.00		NIST Webbook
tb	700.55	K	Joback Method
tc	954.16	K	Joback Method
tf	500.41	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.16	J/mol×K	700.55	Joback Method
cpg	410.80	J/mol×K	742.82	Joback Method
cpg	421.45	J/mol×K	785.09	Joback Method
cpg	431.16	J/mol×K	827.35	Joback Method
cpg	439.96	J/mol×K	869.62	Joback Method
cpg	447.90	J/mol×K	911.89	Joback Method
cpg	455.02	J/mol×K	954.16	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=U299264&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