4-Nitrobenzoic acid, pent-2-en-4-ynyl ester

Inchi: InChI=1S/C12H9NO4/c1-2-3-4-9-17-12(14)10-5-7-11(8-6-10)13(15)16/h1,3-8H,9H2
InchiKey: MXGZFNDFBAXWGJ-UHFFFAOYSA-N
Formula: C12H9NO4
SMILES: C#CC=CCOC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 231.20

Physical Properties

Property code	Value	Unit	Source
gf	257.86	kJ/mol	Joback Method
hf	87.61	kJ/mol	Joback Method
hfus	37.81	kJ/mol	Joback Method
hvap	70.81	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	1.941		Crippen Method
mcvol	168.140	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
rinpol	1839.00		NIST Webbook
rinpol	1839.00		NIST Webbook
tb	728.03	K	Joback Method
tc	980.95	K	Joback Method
tf	521.60	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.37	J/mol×K	728.03	Joback Method
cpg	435.65	J/mol×K	770.18	Joback Method
cpg	445.99	J/mol×K	812.34	Joback Method
cpg	455.45	J/mol×K	854.49	Joback Method
cpg	464.10	J/mol×K	896.64	Joback Method
cpg	472.02	J/mol×K	938.80	Joback Method
cpg	479.27	J/mol×K	980.95	Joback Method

Sources

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=U299266&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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