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

Inchi: InChI=1S/C13H13NO4/c1-3-5-12(4-2)18-13(15)10-6-8-11(9-7-10)14(16)17/h6-9,12H,4H2
InchiKey: KLQGTLNYSZNHAU-UHFFFAOYSA-N
Formula: C13H13NO4
SMILES: CC#CC(CC)OC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 247.25

Physical Properties

Property code	Value	Unit	Source
gf	163.35	kJ/mol	Joback Method
hf	-75.13	kJ/mol	Joback Method
hfus	36.82	kJ/mol	Joback Method
hvap	74.98	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	2.554		Crippen Method
mcvol	186.530	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
rinpol	1857.00		NIST Webbook
rinpol	1857.00		NIST Webbook
tb	765.19	K	Joback Method
tc	1017.91	K	Joback Method
tf	582.08	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.01	J/mol×K	765.19	Joback Method
cpg	515.18	J/mol×K	807.31	Joback Method
cpg	527.22	J/mol×K	849.43	Joback Method
cpg	538.18	J/mol×K	891.55	Joback Method
cpg	548.08	J/mol×K	933.67	Joback Method
cpg	556.95	J/mol×K	975.79	Joback Method
cpg	564.85	J/mol×K	1017.91	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=U299267&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