Benzeneacetic acid, 4-nitro-, hex-4-yn-3-yl ester

Inchi: InChI=1S/C14H15NO4/c1-3-5-13(4-2)19-14(16)10-11-6-8-12(9-7-11)15(17)18/h6-9,13H,
InchiKey: CWTZQCPCVHRDLA-UHFFFAOYSA-N
Formula: C14H15NO4
SMILES: CC#CC(CC)OC(=O)Cc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 261.27

Physical Properties

Property code	Value	Unit	Source
gf	171.77	kJ/mol	Joback Method
hf	-95.77	kJ/mol	Joback Method
hfus	39.41	kJ/mol	Joback Method
hvap	77.21	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	2.482		Crippen Method
mcvol	200.620	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	2061.00		NIST Webbook
rinpol	2061.00		NIST Webbook
tb	788.07	K	Joback Method
tc	1035.55	K	Joback Method
tf	593.35	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.31	J/mol×K	788.07	Joback Method
cpg	568.86	J/mol×K	829.32	Joback Method
cpg	581.27	J/mol×K	870.56	Joback Method
cpg	592.57	J/mol×K	911.81	Joback Method
cpg	602.81	J/mol×K	953.06	Joback Method
cpg	612.01	J/mol×K	994.30	Joback Method
cpg	620.22	J/mol×K	1035.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406977&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