Benzeneacetic acid, 4-nitro-, 2,7-dimethyloct-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C18H21NO4/c1-13(2)5-10-17(11-14(3)4)23-18(20)12-15-6-8-16(9-7-15)19(21)

InchiKey: WSVRONZAOIKFHC-UHFFFAOYSA-N

Formula: C18H21NO4

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

Mol. weight [g/mol]: 315.36

Physical Properties

Property code	Value	Unit	Source
gf	282.30	kJ/mol	Joback Method
hf	-67.97	kJ/mol	Joback Method
hfus	43.66	kJ/mol	Joback Method
hvap	85.13	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	3.675		Crippen Method
mcvol	252.680	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
rinpol	2284.00		NIST Webbook
tb	875.71	K	Joback Method
tc	1117.79	K	Joback Method
tf	607.71	K	Joback Method
vc	0.974	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.97	J/mol×K	875.71	Joback Method
cpg	765.32	J/mol×K	916.06	Joback Method
cpg	778.45	J/mol×K	956.40	Joback Method
cpg	790.41	J/mol×K	996.75	Joback Method
cpg	801.26	J/mol×K	1037.10	Joback Method
cpg	811.08	J/mol×K	1077.45	Joback Method
cpg	819.91	J/mol×K	1117.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406980&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