4-Nitrobenzoic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

Inchi: InChI=1S/C17H19NO4/c1-12(2)5-10-16(11-13(3)4)22-17(19)14-6-8-15(9-7-14)18(20)21/

InchiKey: RUYNTJYQYZBXQH-UHFFFAOYSA-N

Formula: C17H19NO4

SMILES: C=C(C)C#CC(CC(C)C)OC(=O)c1ccc([N+](=O)[O-])cc1

Mol. weight [g/mol]: 301.34

Physical Properties

Property code	Value	Unit	Source
gf	273.88	kJ/mol	Joback Method
hf	-47.33	kJ/mol	Joback Method
hfus	41.07	kJ/mol	Joback Method
hvap	82.91	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	3.746		Crippen Method
mcvol	238.590	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	2107.00		NIST Webbook
tb	852.83	K	Joback Method
tc	1098.78	K	Joback Method
tf	596.44	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	694.34	J/mol×K	852.83	Joback Method
cpg	708.53	J/mol×K	893.82	Joback Method
cpg	721.49	J/mol×K	934.81	Joback Method
cpg	733.29	J/mol×K	975.80	Joback Method
cpg	743.98	J/mol×K	1016.79	Joback Method
cpg	753.63	J/mol×K	1057.78	Joback Method
cpg	762.28	J/mol×K	1098.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299270&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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