4-Nitrobenzoic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C16H19NO4/c1-4-5-6-15(11-12(2)3)21-16(18)13-7-9-14(10-8-13)17(19)20/h7-1

InchiKey: SFNNMCIJIXGXOM-UHFFFAOYSA-N

Formula: C16H19NO4

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

Mol. weight [g/mol]: 289.33

Physical Properties

Property code	Value	Unit	Source
gf	186.17	kJ/mol	Joback Method
hf	-142.33	kJ/mol	Joback Method
hfus	41.07	kJ/mol	Joback Method
hvap	81.27	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	3.580		Crippen Method
mcvol	228.800	ml/mol	McGowan Method
pc	2058.62	kPa	Joback Method
rinpol	2060.00		NIST Webbook
rinpol	2060.00		NIST Webbook
tb	833.39	K	Joback Method
tc	1076.04	K	Joback Method
tf	600.89	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.61	J/mol×K	833.39	Joback Method
cpg	679.93	J/mol×K	873.83	Joback Method
cpg	693.03	J/mol×K	914.27	Joback Method
cpg	704.94	J/mol×K	954.72	Joback Method
cpg	715.71	J/mol×K	995.16	Joback Method
cpg	725.38	J/mol×K	1035.60	Joback Method
cpg	734.01	J/mol×K	1076.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299269&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