Benzoic acid, 3,5-dinitro, 2-propynyl ester

Other names: Benzoic acid, 3,5-dinitro, 2-propynyl ester
2-Propynyl 3,5-dinitrobenzoate
Inchi: InChI=1S/C10H6N2O6/c1-2-3-18-10(13)7-4-8(11(14)15)6-9(5-7)12(16)17/h1,4-6H,3H2
InchiKey: YBKJIXGRDWJQTE-UHFFFAOYSA-N
Formula: C10H6N2O6
SMILES: C#CCOC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 250.17

Physical Properties

Property code	Value	Unit	Source
hfus	43.40	kJ/mol	Joback Method
ie	10.50	eV	Cheméo Relay (1.0)
log10ws	-3.78		Cheméo Relay (1.0)
logp	1.293		Crippen Method
mcvol	161.680	ml/mol	McGowan Method
rinpol	1846.00		NIST Webbook
rinpol	1857.00		NIST Webbook
rinpol	1862.00		NIST Webbook
ripol	3094.00		NIST Webbook
ripol	3119.00		NIST Webbook
ripol	3125.00		NIST Webbook
ripol	3105.00		NIST Webbook
tf	353.52	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.83	J/mol×K	834.93	Joback Method
cpg	435.23	J/mol×K	880.16	Joback Method
cpg	442.66	J/mol×K	925.39	Joback Method
cpg	449.17	J/mol×K	970.61	Joback Method
cpg	454.81	J/mol×K	1015.84	Joback Method
cpg	459.61	J/mol×K	1061.07	Joback Method
cpg	463.62	J/mol×K	1106.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373855&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tf:	Normal melting (fusion) point