Prop-2-ynyl 3,5-dinitrobenzoate

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]: 250.16

Physical Properties

Property code	Value	Unit	Source
gf	186.72	kJ/mol	Joback Method
hf	-10.56	kJ/mol	Joback Method
hfus	43.40	kJ/mol	Joback Method
hvap	83.65	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	1.293		Crippen Method
mcvol	161.680	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method
rinpol	1862.00		NIST Webbook
rinpol	1846.00		NIST Webbook
rinpol	1857.00		NIST Webbook
ripol	3094.00		NIST Webbook
ripol	3105.00		NIST Webbook
ripol	3125.00		NIST Webbook
ripol	3119.00		NIST Webbook
tb	834.93	K	Joback Method
tc	1106.30	K	Joback Method
tf	660.27	K	Joback Method
vc	0.637	m3/kmol	Joback Method

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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume