But-3-enyl 3,5-dinitrobenzoate

Other names: Benzoic acid, 3,5-dinitro, 3-butenyl ester
3-Butenyl 3,5-dinitrobenzoate
Inchi: InChI=1S/C11H10N2O6/c1-2-3-4-19-11(14)8-5-9(12(15)16)7-10(6-8)13(17)18/h2,5-7H,1
InchiKey: AUGWZTWOGIRQQN-UHFFFAOYSA-N
Formula: C11H10N2O6
SMILES: C=CCCOC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 266.21

Physical Properties

Property code	Value	Unit	Source
gf	59.91	kJ/mol	Joback Method
hf	-197.67	kJ/mol	Joback Method
hfus	41.74	kJ/mol	Joback Method
hvap	85.35	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	2.236		Crippen Method
mcvol	180.070	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
rinpol	1934.00		NIST Webbook
rinpol	1942.00		NIST Webbook
rinpol	1938.00		NIST Webbook
rinpol	1920.00		NIST Webbook
ripol	2956.00		NIST Webbook
ripol	2935.00		NIST Webbook
ripol	2953.00		NIST Webbook
ripol	2974.00		NIST Webbook
ripol	2935.00		NIST Webbook
tb	864.37	K	Joback Method
tc	1119.11	K	Joback Method
tf	622.81	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.97	J/mol×K	864.37	Joback Method
cpg	516.43	J/mol×K	906.83	Joback Method
cpg	524.87	J/mol×K	949.28	Joback Method
cpg	532.35	J/mol×K	991.74	Joback Method
cpg	538.89	J/mol×K	1034.20	Joback Method
cpg	544.54	J/mol×K	1076.66	Joback Method
cpg	549.35	J/mol×K	1119.11	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373853&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