(E)-But-2-enyl 3,5-dinitrobenzoate

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

Physical Properties

Property code	Value	Unit	Source
gf	52.29	kJ/mol	Joback Method
hf	-205.88	kJ/mol	Joback Method
hfus	43.22	kJ/mol	Joback Method
hvap	85.98	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	2.236		Crippen Method
mcvol	180.070	ml/mol	McGowan Method
pc	2918.68	kPa	Joback Method
rinpol	1970.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	2048.00		NIST Webbook
rinpol	1948.00		NIST Webbook
rinpol	1956.00		NIST Webbook
rinpol	1948.00		NIST Webbook
rinpol	2048.00		NIST Webbook
rinpol	1967.00		NIST Webbook
ripol	2997.00		NIST Webbook
ripol	2997.00		NIST Webbook
ripol	2972.00		NIST Webbook
ripol	2972.00		NIST Webbook
ripol	2989.00		NIST Webbook
ripol	3009.00		NIST Webbook
tb	871.85	K	Joback Method
tc	1130.79	K	Joback Method
tf	619.49	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.00	J/mol×K	871.85	Joback Method
cpg	515.56	J/mol×K	915.01	Joback Method
cpg	524.15	J/mol×K	958.16	Joback Method
cpg	531.84	J/mol×K	1001.32	Joback Method
cpg	538.69	J/mol×K	1044.48	Joback Method
cpg	544.76	J/mol×K	1087.63	Joback Method
cpg	550.09	J/mol×K	1130.79	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373850&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

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