Benzoic acid, 3,5-dinitro, 1-methyl-3-butenyl ester

Other names: 4-Penten-2-yl 3,5-dinitrobenzoate
Inchi: InChI=1S/C12H12N2O6/c1-3-4-8(2)20-12(15)9-5-10(13(16)17)7-11(6-9)14(18)19/h3,5-8H
InchiKey: QXQDHMYXHILXEV-UHFFFAOYSA-N
Formula: C12H12N2O6
SMILES: C=CCC(C)OC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 280.23

Physical Properties

Property code	Value	Unit	Source
gf	65.89	kJ/mol	Joback Method
hf	-223.59	kJ/mol	Joback Method
hfus	40.80	kJ/mol	Joback Method
hvap	87.19	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	2.624		Crippen Method
mcvol	194.160	ml/mol	McGowan Method
pc	2632.55	kPa	Joback Method
rinpol	1962.00		NIST Webbook
rinpol	1940.00		NIST Webbook
rinpol	1940.00		NIST Webbook
rinpol	1951.00		NIST Webbook
rinpol	1962.00		NIST Webbook
rinpol	1961.00		NIST Webbook
ripol	2883.00		NIST Webbook
ripol	2890.00		NIST Webbook
ripol	2866.00		NIST Webbook
ripol	2866.00		NIST Webbook
ripol	2890.00		NIST Webbook
ripol	2905.00		NIST Webbook
tb	886.81	K	Joback Method
tc	1141.14	K	Joback Method
tf	619.08	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.66	J/mol×K	886.81	Joback Method
cpg	571.60	J/mol×K	929.20	Joback Method
cpg	580.46	J/mol×K	971.59	Joback Method
cpg	588.29	J/mol×K	1013.98	Joback Method
cpg	595.13	J/mol×K	1056.36	Joback Method
cpg	601.02	J/mol×K	1098.75	Joback Method
cpg	606.02	J/mol×K	1141.14	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R34721&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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