3-Methylbut-3-enyl 3,5-dinitrobenzoate

Inchi: InChI=1S/C12H12N2O6/c1-8(2)3-4-20-12(15)9-5-10(13(16)17)7-11(6-9)14(18)19/h5-7H,
InchiKey: XGFGKTGBDOKXEY-UHFFFAOYSA-N
Formula: C12H12N2O6
SMILES: C=C(C)CCOC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 280.23

Physical Properties

Property code	Value	Unit	Source
gf	59.78	kJ/mol	Joback Method
hf	-228.10	kJ/mol	Joback Method
hfus	43.02	kJ/mol	Joback Method
hvap	87.65	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	2.626		Crippen Method
mcvol	194.160	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
rinpol	2111.00		NIST Webbook
tb	887.13	K	Joback Method
tc	1140.80	K	Joback Method
tf	620.12	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.72	J/mol×K	887.13	Joback Method
cpg	570.68	J/mol×K	929.41	Joback Method
cpg	579.60	J/mol×K	971.69	Joback Method
cpg	587.52	J/mol×K	1013.96	Joback Method
cpg	594.48	J/mol×K	1056.24	Joback Method
cpg	600.53	J/mol×K	1098.52	Joback Method
cpg	605.72	J/mol×K	1140.80	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373861&Units=SI

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

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