3,3-Dimethylbutan-2-yl 3,5-dinitrobenzoate

Inchi: InChI=1S/C13H16N2O6/c1-8(13(2,3)4)21-12(16)9-5-10(14(17)18)7-11(6-9)15(19)20/h5-8
InchiKey: HAXSCMWRBHTBLA-UHFFFAOYSA-N
Formula: C13H16N2O6
SMILES: CC(OC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1)C(C)(C)C
Mol. weight [g/mol]: 296.28

Physical Properties

Property code	Value	Unit	Source
gf	-10.69	kJ/mol	Joback Method
hf	-378.41	kJ/mol	Joback Method
hfus	37.26	kJ/mol	Joback Method
hvap	88.79	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	3.094		Crippen Method
mcvol	212.550	ml/mol	McGowan Method
pc	2338.29	kPa	Joback Method
rinpol	2073.00		NIST Webbook
rinpol	2073.00		NIST Webbook
tb	909.78	K	Joback Method
tc	1167.22	K	Joback Method
tf	634.53	K	Joback Method
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.65	J/mol×K	909.78	Joback Method
cpg	656.61	J/mol×K	952.69	Joback Method
cpg	666.44	J/mol×K	995.59	Joback Method
cpg	675.22	J/mol×K	1038.50	Joback Method
cpg	683.03	J/mol×K	1081.41	Joback Method
cpg	689.94	J/mol×K	1124.31	Joback Method
cpg	696.03	J/mol×K	1167.22	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=U373876&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