2,4-Dimethylpentan-3-yl 3,5-dinitrobenzoate

Inchi: InChI=1S/C14H18N2O6/c1-8(2)13(9(3)4)22-14(17)10-5-11(15(18)19)7-12(6-10)16(20)21
InchiKey: BVZGIOBDGBDXJU-UHFFFAOYSA-N
Formula: C14H18N2O6
SMILES: CC(C)C(OC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1)C(C)C
Mol. weight [g/mol]: 310.30

Physical Properties

Property code	Value	Unit	Source
gf	-9.99	kJ/mol	Joback Method
hf	-400.86	kJ/mol	Joback Method
hfus	40.22	kJ/mol	Joback Method
hvap	91.53	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	3.340		Crippen Method
mcvol	226.640	ml/mol	McGowan Method
pc	2129.52	kPa	Joback Method
rinpol	2144.00		NIST Webbook
rinpol	2144.00		NIST Webbook
tb	935.01	K	Joback Method
tc	1185.28	K	Joback Method
tf	613.38	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.85	J/mol×K	935.01	Joback Method
cpg	712.95	J/mol×K	976.72	Joback Method
cpg	722.78	J/mol×K	1018.43	Joback Method
cpg	731.40	J/mol×K	1060.15	Joback Method
cpg	738.85	J/mol×K	1101.86	Joback Method
cpg	745.17	J/mol×K	1143.57	Joback Method
cpg	750.42	J/mol×K	1185.28	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=U373875&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