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

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

Physical Properties

Property code	Value	Unit	Source
gf	-15.97	kJ/mol	Joback Method
hf	-374.94	kJ/mol	Joback Method
hfus	41.15	kJ/mol	Joback Method
hvap	89.69	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	3.094		Crippen Method
mcvol	212.550	ml/mol	McGowan Method
pc	2313.61	kPa	Joback Method
rinpol	2091.00		NIST Webbook
rinpol	2091.00		NIST Webbook
tb	912.57	K	Joback Method
tc	1162.75	K	Joback Method
tf	617.11	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.14	J/mol×K	912.57	Joback Method
cpg	655.96	J/mol×K	954.27	Joback Method
cpg	665.59	J/mol×K	995.96	Joback Method
cpg	674.06	J/mol×K	1037.66	Joback Method
cpg	681.41	J/mol×K	1079.36	Joback Method
cpg	687.68	J/mol×K	1121.05	Joback Method
cpg	692.92	J/mol×K	1162.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373878&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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