Hexan-2-yl 3,5-dinitrobenzoate

Inchi: InChI=1S/C13H16N2O6/c1-3-4-5-9(2)21-13(16)10-6-11(14(17)18)8-12(7-10)15(19)20/h6
InchiKey: ZQARXIOVXXLMCF-UHFFFAOYSA-N
Formula: C13H16N2O6
SMILES: CCCCC(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	-13.53	kJ/mol	Joback Method
hf	-369.66	kJ/mol	Joback Method
hfus	44.67	kJ/mol	Joback Method
hvap	90.08	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	3.239		Crippen Method
mcvol	212.550	ml/mol	McGowan Method
pc	2295.91	kPa	Joback Method
rinpol	2140.00		NIST Webbook
tb	913.01	K	Joback Method
tc	1159.53	K	Joback Method
tf	632.11	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.58	J/mol×K	913.01	Joback Method
cpg	655.30	J/mol×K	954.10	Joback Method
cpg	664.87	J/mol×K	995.18	Joback Method
cpg	673.34	J/mol×K	1036.27	Joback Method
cpg	680.72	J/mol×K	1077.36	Joback Method
cpg	687.08	J/mol×K	1118.45	Joback Method
cpg	692.45	J/mol×K	1159.53	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=U373874&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