Octan-2-yl 3,5-dinitrobenzoate

Inchi: InChI=1S/C15H20N2O6/c1-3-4-5-6-7-11(2)23-15(18)12-8-13(16(19)20)10-14(9-12)17(21
InchiKey: DZNKEPDYVBEFSO-UHFFFAOYSA-N
Formula: C15H20N2O6
SMILES: CCCCCCC(C)OC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 324.33

Physical Properties

Property code	Value	Unit	Source
gf	3.31	kJ/mol	Joback Method
hf	-410.94	kJ/mol	Joback Method
hfus	49.85	kJ/mol	Joback Method
hvap	94.53	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	4.019		Crippen Method
mcvol	240.730	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
rinpol	2333.00		NIST Webbook
tb	958.77	K	Joback Method
tc	1200.07	K	Joback Method
tf	654.65	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	757.76	J/mol×K	958.77	Joback Method
cpg	768.84	J/mol×K	998.99	Joback Method
cpg	778.74	J/mol×K	1039.20	Joback Method
cpg	787.50	J/mol×K	1079.42	Joback Method
cpg	795.18	J/mol×K	1119.63	Joback Method
cpg	801.81	J/mol×K	1159.85	Joback Method
cpg	807.45	J/mol×K	1200.07	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=U373877&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