3,7-Dimethyloct-6-enyl 3,5-dinitrobenzoate

Inchi: InChI=1S/C17H22N2O6/c1-12(2)5-4-6-13(3)7-8-25-17(20)14-9-15(18(21)22)11-16(10-14
InchiKey: HEVIMRBTPATVSL-UHFFFAOYSA-N
Formula: C17H22N2O6
SMILES: CC(C)=CCCC(C)CCOC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 350.37

Physical Properties

Property code	Value	Unit	Source
gf	91.82	kJ/mol	Joback Method
hf	-344.79	kJ/mol	Joback Method
hfus	53.93	kJ/mol	Joback Method
hvap	99.02	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	4.432		Crippen Method
mcvol	264.610	ml/mol	McGowan Method
pc	1716.03	kPa	Joback Method
rinpol	2580.00		NIST Webbook
rinpol	2580.00		NIST Webbook
tb	1008.57	K	Joback Method
tc	1254.70	K	Joback Method
tf	658.15	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.97	J/mol×K	1008.57	Joback Method
cpg	855.45	J/mol×K	1049.59	Joback Method
cpg	865.87	J/mol×K	1090.61	Joback Method
cpg	875.33	J/mol×K	1131.64	Joback Method
cpg	883.89	J/mol×K	1172.66	Joback Method
cpg	891.64	J/mol×K	1213.68	Joback Method
cpg	898.65	J/mol×K	1254.70	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=U373862&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