Neopentyl 3,5-dinitrobenzoate

Inchi: InChI=1S/C12H14N2O6/c1-12(2,3)7-20-11(15)8-4-9(13(16)17)6-10(5-8)14(18)19/h4-6H,
InchiKey: KTDNZFJHYUNSJU-UHFFFAOYSA-N
Formula: C12H14N2O6
SMILES: CC(C)(C)COC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 282.25

Physical Properties

Property code	Value	Unit	Source
gf	-16.67	kJ/mol	Joback Method
hf	-352.49	kJ/mol	Joback Method
hfus	38.19	kJ/mol	Joback Method
hvap	86.95	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	2.706		Crippen Method
mcvol	198.460	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
rinpol	2010.00		NIST Webbook
rinpol	2010.00		NIST Webbook
tb	887.34	K	Joback Method
tc	1145.22	K	Joback Method
tf	638.26	K	Joback Method
vc	0.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.87	J/mol×K	887.34	Joback Method
cpg	600.42	J/mol×K	930.32	Joback Method
cpg	609.89	J/mol×K	973.30	Joback Method
cpg	618.35	J/mol×K	1016.28	Joback Method
cpg	625.88	J/mol×K	1059.26	Joback Method
cpg	632.55	J/mol×K	1102.24	Joback Method
cpg	638.44	J/mol×K	1145.22	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=U373848&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