1,7,7-Trimethylbicyclo[2.2.1]heptan-2-yl 3,5-dinitrobenzoate

Inchi: InChI=1S/C17H20N2O6/c1-16(2)11-4-5-17(16,3)14(8-11)25-15(20)10-6-12(18(21)22)9-1

InchiKey: QOMUVRIFQWSYPD-UHFFFAOYSA-N

Formula: C17H20N2O6

SMILES: CC1(C)C2CCC1(C)C(OC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1)C2

Mol. weight [g/mol]: 348.35

CAS: 892105-21-4

Physical Properties

Property code	Value	Unit	Source
gf	105.59	kJ/mol	Joback Method
hf	-317.70	kJ/mol	Joback Method
hfus	42.27	kJ/mol	Joback Method
hvap	96.45	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	3.875		Crippen Method
mcvol	247.190	ml/mol	McGowan Method
pc	2123.64	kPa	Joback Method
rinpol	2598.00		NIST Webbook
tb	1013.86	K	Joback Method
tc	1285.51	K	Joback Method
tf	763.87	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	868.77	J/mol×K	1013.86	Joback Method
cpg	895.41	J/mol×K	1059.14	Joback Method
cpg	924.22	J/mol×K	1104.41	Joback Method
cpg	955.67	J/mol×K	1149.69	Joback Method
cpg	990.25	J/mol×K	1194.96	Joback Method
cpg	1028.42	J/mol×K	1240.24	Joback Method
cpg	1070.65	J/mol×K	1285.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C892105214&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

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