3-Oxobutan-2-yl 3,5-dinitrobenzoate

Inchi: InChI=1S/C11H10N2O7/c1-6(14)7(2)20-11(15)8-3-9(12(16)17)5-10(4-8)13(18)19/h3-5,7H
InchiKey: PUMPIKDMGFQJIX-UHFFFAOYSA-N
Formula: C11H10N2O7
SMILES: CC(=O)C(C)OC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 282.21

Physical Properties

Property code	Value	Unit	Source
gf	-159.29	kJ/mol	Joback Method
hf	-440.96	kJ/mol	Joback Method
hfus	41.09	kJ/mol	Joback Method
hvap	92.38	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	1.637		Crippen Method
mcvol	185.940	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
rinpol	2127.00		NIST Webbook
tb	921.12	K	Joback Method
tc	1179.97	K	Joback Method
tf	659.50	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.68	J/mol×K	921.12	Joback Method
cpg	545.85	J/mol×K	964.26	Joback Method
cpg	552.89	J/mol×K	1007.40	Joback Method
cpg	558.82	J/mol×K	1050.54	Joback Method
cpg	563.67	J/mol×K	1093.69	Joback Method
cpg	567.48	J/mol×K	1136.83	Joback Method
cpg	570.27	J/mol×K	1179.97	Joback Method

Sources

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=U373851&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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