Benzoic acid, 3,5-dinitro, 1-phenylethyl ester

Inchi: InChI=1S/C15H12N2O6/c1-10(11-5-3-2-4-6-11)23-15(18)12-7-13(16(19)20)9-14(8-12)17
InchiKey: YATKDADIXNBBCZ-UHFFFAOYSA-N
Formula: C15H12N2O6
SMILES: CC(OC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1)c1ccccc1
Mol. weight [g/mol]: 316.27

Physical Properties

Property code	Value	Unit	Source
gf	115.72	kJ/mol	Joback Method
hf	-174.41	kJ/mol	Joback Method
hfus	43.90	kJ/mol	Joback Method
hvap	96.81	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	3.421		Crippen Method
mcvol	216.970	ml/mol	McGowan Method
pc	2635.25	kPa	Joback Method
rinpol	2344.00		NIST Webbook
rinpol	2327.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2370.00		NIST Webbook
rinpol	2362.00		NIST Webbook
rinpol	2377.00		NIST Webbook
rinpol	2358.00		NIST Webbook
rinpol	2362.00		NIST Webbook
tb	985.45	K	Joback Method
tc	1260.43	K	Joback Method
tf	681.07	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.67	J/mol×K	985.45	Joback Method
cpg	656.37	J/mol×K	1031.28	Joback Method

cpg	663.79	J/mol×K	1077.11	Joback Method
cpg	670.00	J/mol×K	1122.94	Joback Method
cpg	675.09	J/mol×K	1168.77	Joback Method
cpg	679.15	J/mol×K	1214.60	Joback Method
cpg	682.25	J/mol×K	1260.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R35068&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