Benzoic acid, 3,5-dinitro, 2-phenylethyl ester

Inchi: InChI=1S/C15H12N2O6/c18-15(23-7-6-11-4-2-1-3-5-11)12-8-13(16(19)20)10-14(9-12)17
InchiKey: YGOZXWGXCINERK-UHFFFAOYSA-N
Formula: C15H12N2O6
SMILES: O=C(OCCc1ccccc1)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 316.27

Physical Properties

Property code	Value	Unit	Source
gf	118.16	kJ/mol	Joback Method
hf	-169.13	kJ/mol	Joback Method
hfus	47.42	kJ/mol	Joback Method
hvap	97.20	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	2.902		Crippen Method
mcvol	216.970	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
rinpol	2460.00		NIST Webbook
rinpol	2420.00		NIST Webbook
rinpol	2439.00		NIST Webbook
rinpol	2399.00		NIST Webbook
rinpol	2443.00		NIST Webbook
rinpol	2460.00		NIST Webbook
rinpol	2383.00		NIST Webbook
rinpol	2460.00		NIST Webbook
rinpol	2443.00		NIST Webbook
rinpol	2399.00		NIST Webbook
rinpol	2383.00		NIST Webbook
tb	985.89	K	Joback Method
tc	1256.69	K	Joback Method
tf	696.07	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.20	J/mol×K	985.89	Joback Method
cpg	655.86	J/mol×K	1031.02	Joback Method
cpg	663.29	J/mol×K	1076.16	Joback Method
cpg	669.57	J/mol×K	1121.29	Joback Method
cpg	674.78	J/mol×K	1166.42	Joback Method
cpg	679.01	J/mol×K	1211.56	Joback Method
cpg	682.32	J/mol×K	1256.69	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=R34892&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

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