Benzoic acid, 3,5-dinitro-, phenylmethyl ester

Other names:	Benzyl 3,5-dinitrobenzoate
	Benzoic acid, 3,5-dinitro, benzyl ester
Inchi:	InChI=1S/C14H10N2O6/c17-14(22-9-10-4-2-1-3-5-10)11-6-12(15(18)19)8-13(7-11)16(20
InchiKey:	ULVFRRGXEDYWEM-UHFFFAOYSA-N
Formula:	C14H10N2O6
SMILES:	O=C(OCc1ccccc1)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]:	302.24
CAS:	10478-07-6

Physical Properties

Property code	Value	Unit	Source
gf	109.74	kJ/mol	Joback Method
hf	-148.49	kJ/mol	Joback Method
hfus	44.83	kJ/mol	Joback Method
hvap	94.97	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	2.860		Crippen Method
mcvol	202.880	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	2325.00		NIST Webbook
rinpol	2368.00		NIST Webbook
rinpol	2358.00		NIST Webbook
rinpol	2342.00		NIST Webbook
rinpol	2358.00		NIST Webbook
rinpol	2325.00		NIST Webbook
rinpol	2325.00		NIST Webbook
rinpol	2377.00		NIST Webbook
rinpol	2357.00		NIST Webbook
tb	963.01	K	Joback Method
tc	1238.81	K	Joback Method
tf	684.80	K	Joback Method
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.56	J/mol×K	963.01	Joback Method
cpg	600.00	J/mol×K	1008.98	Joback Method
cpg	607.20	J/mol×K	1054.94	Joback Method
cpg	613.25	J/mol×K	1100.91	Joback Method
cpg	618.21	J/mol×K	1146.88	Joback Method
cpg	622.17	J/mol×K	1192.85	Joback Method
cpg	625.19	J/mol×K	1238.81	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10478076&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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