

Bis-(m,m'-nitrobenzil)

Inchi:	InChI=1S/C14H8N2O6/c17-13(9-3-1-5-11(7-9)15(19)20)14(18)10-4-2-6-12(8-10)16(21)2
InchiKey:	SGKVXDKTNJHBCA-UHFFFAOYSA-N
Formula:	C14H8N2O6
SMILES:	O=C(C(=O)c1cccc([N+](=O)[O-])c1)c1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	300.22
CAS:	5913-06-4

Physical Properties

Property code	Value	Unit	Source
gf	85.82	kJ/mol	Joback Method
hf	-128.85	kJ/mol	Joback Method
hfus	45.24	kJ/mol	Joback Method
hvap	99.31	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	2.569		Crippen Method
mcvol	198.580	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
tb	994.46	K	Joback Method
tc	1277.78	K	Joback Method
tf	712.50	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.06	J/molxK	994.46	Joback Method
cpg	575.34	J/molxK	1041.68	Joback Method
cpg	581.60	J/molxK	1088.90	Joback Method
cpg	586.96	J/molxK	1136.12	Joback Method
cpg	591.52	J/molxK	1183.34	Joback Method
cpg	595.39	J/molxK	1230.56	Joback Method
cpg	598.70	J/molxK	1277.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5913064&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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