BENZOPHENONE, 2-METHYLAMINO-5-NITRO-

Other names: Methanone, [2-(methylamino)-5-nitrophenyl]phenyl-
Benzophenone, 2-methylamino-5-nitro-
2-Methylamino-5-nitrobenzophenone
2-methylamino-5-nitro-benzophenone (MNB)
Inchi: InChI=1S/C14H12N2O3/c1-15-13-8-7-11(16(18)19)9-12(13)14(17)10-5-3-2-4-6-10/h2-9,1
InchiKey: KIWZKBUUWJTGPP-UHFFFAOYSA-N
Formula: C14H12N2O3
SMILES: CNc1ccc([N+](=O)[O-])cc1C(=O)c1ccccc1
Mol. weight [g/mol]: 256.26

Physical Properties

Property code	Value	Unit	Source
hf	26.41	kJ/mol	Cheméo Relay (1.0)
hfus	37.38	kJ/mol	Joback Method
hvap	106.91	kJ/mol	Cheméo Relay (1.0)
ie	8.14	eV	Cheméo Relay (1.0)
log10ws	-3.78		Cheméo Relay (1.0)
logp	2.867		Crippen Method
mcvol	189.570	ml/mol	McGowan Method
rinpol	2390.00		NIST Webbook
rinpol	2378.00		NIST Webbook
rinpol	2390.00		NIST Webbook
tb	634.51	K	Cheméo Relay (1.0)
tf	417.63	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.12	J/mol×K	838.92	Joback Method
cpg	544.78	J/mol×K	882.62	Joback Method
cpg	555.28	J/mol×K	926.33	Joback Method
cpg	564.72	J/mol×K	970.03	Joback Method
cpg	573.17	J/mol×K	1013.74	Joback Method
cpg	580.72	J/mol×K	1057.44	Joback Method

cpg	587.48	J/mol×K	1101.14	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4958569&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point