Benzophenone, 2-(methylamino)-

Inchi: InChI=1S/C14H13NO/c1-15-13-10-6-5-9-12(13)14(16)11-7-3-2-4-8-11/h2-10,15H,1H3
InchiKey: AGKPGIOZNCJFTQ-UHFFFAOYSA-N
Formula: C14H13NO
SMILES: CNc1ccccc1C(=O)c1ccccc1
Mol. weight [g/mol]: 211.26

Physical Properties

Property code	Value	Unit	Source
af	0.5920		Cheméo Relay (1.0)
gf	242.66	kJ/mol	Joback Method
hf	42.03	kJ/mol	Cheméo Relay (1.0)
hfus	26.41	kJ/mol	Joback Method
hvap	96.31	kJ/mol	Cheméo Relay (1.0)
ie	7.79	eV	Cheméo Relay (1.0)
log10ws	-3.43		Cheméo Relay (1.0)
logp	2.959		Crippen Method
mcvol	172.150	ml/mol	McGowan Method
pc	2956.90	kPa	Joback Method
tb	558.20	K	NIST Webbook
tc	897.84	K	Cheméo Relay (1.0)
tf	346.32	K	Cheméo Relay (1.0)
vc	0.614	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.30	J/mol×K	682.10	Joback Method
cpg	455.12	J/mol×K	722.87	Joback Method
cpg	468.73	J/mol×K	763.64	Joback Method
cpg	481.19	J/mol×K	804.41	Joback Method
cpg	492.58	J/mol×K	845.18	Joback Method
cpg	502.98	J/mol×K	885.95	Joback Method
cpg	512.46	J/mol×K	926.72	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	459.20	K	1.60	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1859763&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor
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
ie: Ionization energy
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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume