Methanone, [2-(methylamino)phenyl]phenyl-

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
CAS: 1859-76-3

Physical Properties

Property code	Value	Unit	Source
gf	242.66	kJ/mol	Joback Method
hf	70.19	kJ/mol	Joback Method
hfus	26.41	kJ/mol	Joback Method
hvap	65.15	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
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	926.72	K	Joback Method
tf	415.49	K	Joback Method
vc	0.644	m3/kmol	Joback Method

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:	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=C1859763&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume