2-Buten-1-one, 3-(methylamino)-1-phenyl-

Other names: Crotonophenone, 3-(methylamino)-
3-(Methylamino)-1-phenyl-2-buten-1-one
3-(Methylamino)-1-phenyl-but-2-enone
(E)-3-(Methylamino)-1-phenyl-but-2-enone
Inchi: InChI=1S/C11H13NO/c1-9(12-2)8-11(13)10-6-4-3-5-7-10/h3-8,12H,1-2H3/b9-8+
InchiKey: AYAHPVFYLSWGGO-CMDGGOBGSA-N
Formula: C11H13NO
SMILES: CNC(C)=CC(=O)c1ccccc1
Mol. weight [g/mol]: 175.23
CAS: 14091-93-1

Physical Properties

Property code	Value	Unit	Source
chs	-6033.60 ± 1.50	kJ/mol	NIST Webbook
gf	186.29	kJ/mol	Joback Method
hf	-53.70 ± 4.70	kJ/mol	NIST Webbook
hfs	-152.90 ± 2.10	kJ/mol	NIST Webbook
hfus	23.88	kJ/mol	Joback Method
hsub	99.20 ± 4.20	kJ/mol	NIST Webbook
hsub	99.20 ± 4.20	kJ/mol	NIST Webbook
hvap	55.58	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	1.993		Crippen Method
mcvol	149.340	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
tb	585.84	K	Joback Method
tc	810.72	K	Joback Method
tf	323.70	K	Joback Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.04	J/mol×K	585.84	Joback Method

cpg	365.28	J/mol×K	623.32	Joback Method
cpg	378.53	J/mol×K	660.80	Joback Method
cpg	390.84	J/mol×K	698.28	Joback Method
cpg	402.28	J/mol×K	735.76	Joback Method
cpg	412.90	J/mol×K	773.24	Joback Method
cpg	422.77	J/mol×K	810.72	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14091931&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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