2-Buten-1-one, 3-amino-1-phenyl-

Other names: Crotonophenone, 3-amino-
3-Amino-1-phenyl-but-2-enone
Inchi: InChI=1S/C10H11NO/c1-8(11)7-10(12)9-5-3-2-4-6-9/h2-7H,11H2,1H3/b8-7+
InchiKey: GHPWHAXKMNDINZ-BQYQJAHWSA-N
Formula: C10H11NO
SMILES: CC(N)=CC(=O)c1ccccc1
Mol. weight [g/mol]: 161.20
CAS: 1128-85-4

Physical Properties

Property code	Value	Unit	Source
gf	154.93	kJ/mol	Joback Method
hf	15.44	kJ/mol	Joback Method
hfus	21.39	kJ/mol	Joback Method
hsub	109.40 ± 2.10	kJ/mol	NIST Webbook
hvap	57.55	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	1.732		Crippen Method
mcvol	135.250	ml/mol	McGowan Method
pc	3585.64	kPa	Joback Method
tb	585.32	K	Joback Method
tc	823.93	K	Joback Method
tf	343.03	K	Joback Method
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.59	J/mol×K	585.32	Joback Method
cpg	326.71	J/mol×K	625.09	Joback Method
cpg	338.83	J/mol×K	664.86	Joback Method
cpg	350.02	J/mol×K	704.63	Joback Method
cpg	360.35	J/mol×K	744.39	Joback Method
cpg	369.89	J/mol×K	784.16	Joback Method

cpg	378.70	J/mol×K	823.93	Joback Method

Sources

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=C1128854&Units=SI
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
gf:	Standard Gibbs free energy of formation
hf:	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