Cathinone

Other names:	Norephedrone
	1-Propanone, 2-amino-1-phenyl-, (S)-
	l-Cathinone
	(S)-2-Aminopropiophenone
	(-)-«alpha»-Aminopropiophenone
	S(-)-Cathinone
	2-Amino-1-phenyl-1-propanone
Inchi:	InChI=1S/C9H11NO/c1-7(10)9(11)8-5-3-2-4-6-8/h2-7H,10H2,1H3
InchiKey:	PUAQLLVFLMYYJJ-UHFFFAOYSA-N
Formula:	C9H11NO
SMILES:	CC(N)C(=O)c1ccccc1
Mol. weight [g/mol]:	149.19
CAS:	71031-15-7

Physical Properties

Property code	Value	Unit	Source
gf	72.40	kJ/mol	Joback Method
hf	-76.63	kJ/mol	Joback Method
hfus	16.38	kJ/mol	Joback Method
hvap	54.90	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	1.217		Crippen Method
mcvol	125.460	ml/mol	McGowan Method
pc	3796.32	kPa	Joback Method
rinpol	1334.70		NIST Webbook
rinpol	1334.70		NIST Webbook
tb	557.96	K	Joback Method
tc	791.45	K	Joback Method
tf	335.80	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	288.27	J/mol×K	557.96	Joback Method
cpg	301.36	J/mol×K	596.88	Joback Method
cpg	313.54	J/mol×K	635.79	Joback Method
cpg	324.83	J/mol×K	674.71	Joback Method
cpg	335.28	J/mol×K	713.62	Joback Method
cpg	344.94	J/mol×K	752.54	Joback Method
cpg	353.85	J/mol×K	791.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71031157&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume