

METHCATHINONE

Other names:	1-Propanone, 2-(methylamino)-1-phenyl- 2-(methylamino)propiofenone 2-Methylamino-1-phenylpropanone Cat Ephedrone «alpha»-Methylaminopropiofenone
Inchi:	InChI=1S/C10H13NO/c1-8(11-2)10(12)9-6-4-3-5-7-9/h3-8,11H,1-2H3
InchiKey:	LPLLVINFLBSFRP-UHFFFAOYSA-N
Formula:	C10H13NO
SMILES:	CNC(C)C(=O)c1ccccc1
Mol. weight [g/mol]:	163.22

Physical Properties

Property code	Value	Unit	Source
af	0.4573		Cheméo Relay (1.0)
gf	103.76	kJ/mol	Joback Method
hf	-64.89	kJ/mol	Cheméo Relay (1.0)
hfus	18.87	kJ/mol	Joback Method
hvap	69.04	kJ/mol	Cheméo Relay (1.0)
ie	8.48	eV	Cheméo Relay (1.0)
log10ws	-0.72		Cheméo Relay (1.0)
logp	1.477		Crippen Method
mcvol	139.550	ml/mol	McGowan Method
pc	3217.33	kPa	Joback Method
tb	517.35	K	Cheméo Relay (1.0)
tc	737.41	K	Cheméo Relay (1.0)
tf	368.45	K	Cheméo Relay (1.0)
vc	0.497	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.29	J/mol×K	558.48	Joback Method
cpg	338.54	J/mol×K	595.12	Joback Method

cpg	351.86	J/mol×K	631.77	Joback Method
cpg	364.30	J/mol×K	668.41	Joback Method
cpg	375.89	J/mol×K	705.06	Joback Method
cpg	386.67	J/mol×K	741.70	Joback Method
cpg	396.68	J/mol×K	778.35	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C5650442&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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