

R(+)-Methcathinone

Inchi:	InChI=1S/C10H13NO/c1-8(11-2)10(12)9-6-4-3-5-7-9/h3-8,11H,1-2H3/t8-/m0/s1
InchiKey:	LPLLVINFLBSFRP-QMMMGPBSA-N
Formula:	C10H13NO
SMILES:	CNC(C)C(=O)c1ccccc1
Mol. weight [g/mol]:	163.22
CAS:	160977-88-8

Physical Properties

Property code	Value	Unit	Source
gf	103.76	kJ/mol	Joback Method
hf	-77.59	kJ/mol	Joback Method
hfus	18.87	kJ/mol	Joback Method
hvap	52.92	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	1.477		Crippen Method
mcvol	139.550	ml/mol	McGowan Method
pc	3217.33	kPa	Joback Method
rinpol	1369.90		NIST Webbook
tb	558.48	K	Joback Method
tc	778.35	K	Joback Method
tf	316.47	K	Joback Method
vc	0.522	m3/kmol	Joback Method

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

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=C160977888&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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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