

4-Methylethcathinone

Inchi:	InChI=1S/C12H17NO/c1-4-13-10(3)12(14)11-7-5-9(2)6-8-11/h5-8,10,13H,4H2,1-3H3
InchiKey:	ZOXZWYWOECCBSH-UHFFFAOYSA-N
Formula:	C12H17NO
SMILES:	CCNC(C)C(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	191.27
CAS:	1225617-18-4

Physical Properties

Property code	Value	Unit	Source
gf	110.97	kJ/mol	Joback Method
hf	-130.34	kJ/mol	Joback Method
hfus	23.66	kJ/mol	Joback Method
hvap	58.04	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.176		Crippen Method
mcvol	167.730	ml/mol	McGowan Method
pc	2576.72	kPa	Joback Method
rinpol	1535.10		NIST Webbook
tb	609.22	K	Joback Method
tc	822.57	K	Joback Method
tf	351.53	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.02	J/mol×K	609.22	Joback Method
cpg	435.36	J/mol×K	644.78	Joback Method
cpg	449.76	J/mol×K	680.34	Joback Method
cpg	463.27	J/mol×K	715.89	Joback Method
cpg	475.92	J/mol×K	751.45	Joback Method
cpg	487.74	J/mol×K	787.01	Joback Method
cpg	498.77	J/mol×K	822.57	Joback Method

Sources

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=C1225617184&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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