3,4-Dimethylmethcathinone

Inchi: InChI=1S/C12H17NO/c1-8-5-6-11(7-9(8)2)12(14)10(3)13-4/h5-7,10,13H,1-4H3
InchiKey: IBZRXTVDTGVBIS-UHFFFAOYSA-N
Formula: C12H17NO
SMILES: CNC(C)C(=O)c1ccc(C)c(C)c1
Mol. weight [g/mol]: 191.27
CAS: 1082110-00-6

Physical Properties

Property code	Value	Unit	Source
gf	101.34	kJ/mol	Joback Method
hf	-141.81	kJ/mol	Joback Method
hfus	23.27	kJ/mol	Joback Method
hvap	58.70	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	2.094		Crippen Method
mcvol	167.730	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
rinpol	1602.80		NIST Webbook
rinpol	1602.80		NIST Webbook
tb	614.20	K	Joback Method
tc	828.49	K	Joback Method
tf	364.05	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.51	J/mol×K	614.20	Joback Method
cpg	434.62	J/mol×K	649.92	Joback Method
cpg	448.84	J/mol×K	685.63	Joback Method
cpg	462.19	J/mol×K	721.35	Joback Method
cpg	474.72	J/mol×K	757.06	Joback Method
cpg	486.45	J/mol×K	792.78	Joback Method
cpg	497.42	J/mol×K	828.49	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=C1082110006&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume