

Mephedrone, Ac

Inchi:	InChI=1S/C13H17NO2/c1-9-5-7-12(8-6-9)13(16)10(2)14(4)11(3)15/h5-8,10H,1-4H3
InchiKey:	WILMIIORFNUDME-UHFFFAOYSA-N
Formula:	C13H17NO2
SMILES:	CC(=O)N(C)C(C)C(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	219.28

Physical Properties

Property code	Value	Unit	Source
gf	11.86	kJ/mol	Joback Method
hf	-249.50	kJ/mol	Joback Method
hfus	25.77	kJ/mol	Joback Method
hvap	62.62	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.045		Crippen Method
mcvol	183.390	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
rinpola	1915.00		NIST Webbook
rinpola	1915.00		NIST Webbook
tb	648.24	K	Joback Method
tc	862.51	K	Joback Method
tf	392.54	K	Joback Method
vc	0.679	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.35	J/mol×K	648.24	Joback Method
cpg	489.49	J/mol×K	683.95	Joback Method
cpg	503.63	J/mol×K	719.66	Joback Method
cpg	516.82	J/mol×K	755.37	Joback Method
cpg	529.11	J/mol×K	791.08	Joback Method
cpg	540.52	J/mol×K	826.80	Joback Method
cpg	551.11	J/mol×K	862.51	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R615806&Units=SI

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

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