N-acetyl-3,4-methylenedioxymethcathinone

Other names: N-acetylmethylone
Methylone, Ac
Inchi: InChI=1S/C13H15NO4/c1-8(14(3)9(2)15)13(16)10-4-5-11-12(6-10)18-7-17-11/h4-6,8H,7
InchiKey: SFBOFEWMUYVYDF-UHFFFAOYSA-N
Formula: C13H15NO4
SMILES: CC(=O)N(C)C(C)C(=O)c1ccc2c(c1)OCO2
Mol. weight [g/mol]: 249.26

Physical Properties

Property code	Value	Unit	Source
gf	-101.55	kJ/mol	Joback Method
hf	-431.83	kJ/mol	Joback Method
hfus	38.41	kJ/mol	Joback Method
hvap	72.52	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	1.465		Crippen Method
mcvol	184.270	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
rinpol	1950.00		NIST Webbook
rinpol	1950.00		NIST Webbook
tb	718.53	K	Joback Method
tc	942.77	K	Joback Method
tf	480.38	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.63	J/mol×K	718.53	Joback Method
cpg	527.86	J/mol×K	755.90	Joback Method
cpg	540.12	J/mol×K	793.28	Joback Method
cpg	551.51	J/mol×K	830.65	Joback Method
cpg	562.08	J/mol×K	868.03	Joback Method
cpg	571.93	J/mol×K	905.40	Joback Method

cpg	581.13	J/mol×K	942.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U379025&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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