Methylone M (demethylenyl, 3-O-methyl, nor), 2Ac

Inchi: InChI=1S/C14H17NO5/c1-8(15-9(2)16)14(18)11-5-6-12(20-10(3)17)13(7-11)19-4/h5-8H,

InchiKey: NZDJVZBBLUFYRS-UHFFFAOYSA-N

Formula: C14H17NO5

SMILES: COc1cc(C(=O)C(C)NC(C)=O)ccc1OC(C)=O

Mol. weight [g/mol]: 279.29

Physical Properties

Property code	Value	Unit	Source
gf	-349.66	kJ/mol	Joback Method
hf	-672.69	kJ/mol	Joback Method
hfus	34.03	kJ/mol	Joback Method
hvap	81.46	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	1.328		Crippen Method
mcvol	210.790	ml/mol	McGowan Method
pc	2300.32	kPa	Joback Method
rinpol	1990.00		NIST Webbook
rinpol	1990.00		NIST Webbook
tb	812.54	K	Joback Method
tc	1029.12	K	Joback Method
tf	530.91	K	Joback Method
vc	0.794	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.39	J/mol×K	812.54	Joback Method
cpg	618.59	J/mol×K	848.64	Joback Method
cpg	629.75	J/mol×K	884.73	Joback Method
cpg	639.88	J/mol×K	920.83	Joback Method
cpg	648.98	J/mol×K	956.93	Joback Method
cpg	657.04	J/mol×K	993.02	Joback Method
cpg	664.07	J/mol×K	1029.12	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R615886&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
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