Methylone M (demethylenyl, 3-O-methyl), 2Ac

Inchi: InChI=1S/C15H19NO5/c1-9(16(4)10(2)17)15(19)12-6-7-13(21-11(3)18)14(8-12)20-5/h6-9
InchiKey: IDTQPTVNIJKOCS-UHFFFAOYSA-N
Formula: C15H19NO5
SMILES: COc1cc(C(=O)C(C)N(C)C(C)=O)ccc1OC(C)=O
Mol. weight [g/mol]: 293.32

Physical Properties

Property code	Value	Unit	Source
gf	-319.85	kJ/mol	Joback Method
hf	-679.27	kJ/mol	Joback Method
hfus	34.54	kJ/mol	Joback Method
hvap	79.30	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	1.670		Crippen Method
mcvol	224.880	ml/mol	McGowan Method
pc	2073.65	kPa	Joback Method
rinpol	2045.00		NIST Webbook
rinpol	2045.00		NIST Webbook
tb	797.69	K	Joback Method
tc	1009.68	K	Joback Method
tf	521.99	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.88	J/mol×K	797.69	Joback Method
cpg	662.21	J/mol×K	833.02	Joback Method
cpg	674.48	J/mol×K	868.35	Joback Method
cpg	685.73	J/mol×K	903.69	Joback Method
cpg	695.95	J/mol×K	939.02	Joback Method
cpg	705.15	J/mol×K	974.35	Joback Method
cpg	713.36	J/mol×K	1009.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R615871&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

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