Mephedrone M (Ar-CH2OH, nor), 2Ac

Inchi: InChI=1S/C14H17NO4/c1-9(15-10(2)16)14(18)13-6-4-12(5-7-13)8-19-11(3)17/h4-7,9H,8
InchiKey: PACJGKJARDXWGO-UHFFFAOYSA-N
Formula: C14H17NO4
SMILES: CC(=O)NC(C)C(=O)c1ccc(COC(C)=O)cc1
Mol. weight [g/mol]: 263.29

Physical Properties

Property code	Value	Unit	Source
gf	-235.03	kJ/mol	Joback Method
hf	-529.00	kJ/mol	Joback Method
hfus	33.23	kJ/mol	Joback Method
hvap	78.39	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	1.457		Crippen Method
mcvol	204.920	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook
tb	785.14	K	Joback Method
tc	1002.42	K	Joback Method
tf	496.16	K	Joback Method
vc	0.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.78	J/mol×K	785.14	Joback Method
cpg	594.48	J/mol×K	821.35	Joback Method
cpg	606.19	J/mol×K	857.57	Joback Method
cpg	616.92	J/mol×K	893.78	Joback Method
cpg	626.70	J/mol×K	929.99	Joback Method
cpg	635.56	J/mol×K	966.21	Joback Method
cpg	643.53	J/mol×K	1002.42	Joback Method

Sources

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=R615831&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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