Mephedrone M (Ar-carboxy, dihydro), 3Ac

Inchi: InChI=1S/C17H21NO6/c1-9(18(5)11(3)20)16(24-12(4)21)14-7-6-13(17(22)23)8-15(14)10
InchiKey: OWLXLIYMSCQNHM-UHFFFAOYSA-N
Formula: C17H21NO6
SMILES: CC(=O)OC(c1ccc(C(=O)O)cc1C(C)=O)C(C)N(C)C(C)=O
Mol. weight [g/mol]: 335.35

Physical Properties

Property code	Value	Unit	Source
gf	-466.19	kJ/mol	Joback Method
hf	-858.42	kJ/mol	Joback Method
hfus	40.70	kJ/mol	Joback Method
hvap	104.38	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.058		Crippen Method
mcvol	254.630	ml/mol	McGowan Method
pc	2051.17	kPa	Joback Method
rinpol	2235.00		NIST Webbook
rinpol	2235.00		NIST Webbook
tb	966.64	K	Joback Method
tc	1187.35	K	Joback Method
tf	618.05	K	Joback Method
vc	0.947	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.06	J/mol×K	966.64	Joback Method
cpg	805.00	J/mol×K	1003.43	Joback Method
cpg	813.87	J/mol×K	1040.21	Joback Method
cpg	821.71	J/mol×K	1077.00	Joback Method
cpg	828.55	J/mol×K	1113.78	Joback Method
cpg	834.44	J/mol×K	1150.57	Joback Method
cpg	839.41	J/mol×K	1187.35	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=R615811&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