Methylenedioxyamphetamine acetate

Other names: N-Acetyl-3,4-methylenedioxyamphetamine
3,4-Methylenedioxyamphetamine, AC
Inchi: InChI=1S/C12H15NO3/c1-8(13-9(2)14)5-10-3-4-11-12(6-10)16-7-15-11/h3-4,6,8H,5,7H2
InchiKey: RSXXYTIHSOOFBG-UHFFFAOYSA-N
Formula: C12H15NO3
SMILES: CC(=O)NC(C)Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]: 221.25
CAS: 36209-71-9

Physical Properties

Property code	Value	Unit	Source
gf	-2.44	kJ/mol	Joback Method
hf	-312.67	kJ/mol	Joback Method
hfus	36.30	kJ/mol	Joback Method
hvap	67.94	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	1.482		Crippen Method
mcvol	168.610	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	1860.00		NIST Webbook
rinpol	1860.00		NIST Webbook
tb	679.51	K	Joback Method
tc	903.50	K	Joback Method
tf	439.37	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.49	J/mol×K	679.51	Joback Method
cpg	475.08	J/mol×K	716.84	Joback Method
cpg	487.72	J/mol×K	754.17	Joback Method
cpg	499.50	J/mol×K	791.50	Joback Method
cpg	510.47	J/mol×K	828.84	Joback Method

cpg	520.70	J/mol×K	866.17	Joback Method
cpg	530.27	J/mol×K	903.50	Joback Method

Sources

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=C36209719&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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