4-Methylthioamphetamine-M (ring-HO-) diacetylated

Inchi: InChI=1S/C14H18O4S/c1-9(17-10(2)15)7-12-5-6-14(19-4)13(8-12)18-11(3)16/h5-6,8-9H
InchiKey: NLMKGRSEWHJTNY-UHFFFAOYSA-N
Formula: C14H18O4S
SMILES: CSc1ccc(CC(C)OC(C)=O)cc1OC(C)=O
Mol. weight [g/mol]: 282.36

Physical Properties

Property code	Value	Unit	Source
gf	-277.01	kJ/mol	Joback Method
hf	-571.71	kJ/mol	Joback Method
hfus	31.46	kJ/mol	Joback Method
hvap	75.10	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	2.828		Crippen Method
mcvol	215.590	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
rinpol	2240.00		NIST Webbook
tb	777.28	K	Joback Method
tc	1001.54	K	Joback Method
tf	462.72	K	Joback Method
vc	0.807	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.80	J/mol×K	777.28	Joback Method
cpg	607.56	J/mol×K	814.66	Joback Method
cpg	620.20	J/mol×K	852.03	Joback Method
cpg	631.72	J/mol×K	889.41	Joback Method
cpg	642.11	J/mol×K	926.79	Joback Method
cpg	651.37	J/mol×K	964.17	Joback Method
cpg	659.47	J/mol×K	1001.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R413264&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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