4-Methylthioamphetamine-M (HO-) diacetlyated

Inchi: InChI=1S/C14H18O4S/c1-9(17-10(2)15)14(18-11(3)16)12-5-7-13(19-4)8-6-12/h5-9,14H,1

InchiKey: XJXRFTAVICFYMU-UHFFFAOYSA-N

Formula: C14H18O4S

SMILES: CSc1ccc(C(OC(C)=O)C(C)OC(C)=O)cc1

Mol. weight [g/mol]: 282.36

Physical Properties

Property code	Value	Unit	Source
gf	-269.82	kJ/mol	Joback Method
hf	-565.52	kJ/mol	Joback Method
hfus	28.33	kJ/mol	Joback Method
hvap	74.05	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	2.964		Crippen Method
mcvol	215.590	ml/mol	McGowan Method
pc	2222.89	kPa	Joback Method
rinpol	2260.00		NIST Webbook
tb	771.86	K	Joback Method
tc	999.12	K	Joback Method
tf	435.20	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.59	J/mol×K	771.86	Joback Method
cpg	609.69	J/mol×K	809.74	Joback Method
cpg	622.61	J/mol×K	847.61	Joback Method
cpg	634.36	J/mol×K	885.49	Joback Method
cpg	644.94	J/mol×K	923.37	Joback Method
cpg	654.34	J/mol×K	961.25	Joback Method
cpg	662.56	J/mol×K	999.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R413244&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