Spermidine, N,N',N''-triacetyl-

Inchi: InChI=1S/C13H25N3O3/c1-11(17)14-7-4-5-9-16(13(3)19)10-6-8-15-12(2)18/h4-10H2,1-3
InchiKey: GDVGUTLRMWMZBV-UHFFFAOYSA-N
Formula: C13H25N3O3
SMILES: CC(=O)NCCCCN(CCCNC(C)=O)C(C)=O
Mol. weight [g/mol]: 271.36

Physical Properties

Property code	Value	Unit	Source
gf	-38.62	kJ/mol	Joback Method
hf	-474.92	kJ/mol	Joback Method
hfus	47.44	kJ/mol	Joback Method
hvap	79.68	kJ/mol	Joback Method
log10ws	-1.54		Crippen Method
logp	0.277		Crippen Method
mcvol	228.680	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	2648.00		NIST Webbook
tb	771.23	K	Joback Method
tc	960.58	K	Joback Method
tf	523.85	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.06	J/mol×K	771.23	Joback Method
cpg	699.90	J/mol×K	802.79	Joback Method
cpg	712.90	J/mol×K	834.35	Joback Method
cpg	725.11	J/mol×K	865.90	Joback Method
cpg	736.56	J/mol×K	897.46	Joback Method
cpg	747.27	J/mol×K	929.02	Joback Method
cpg	757.29	J/mol×K	960.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352599&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