Spermidine, N-isoBOC, O-TBDMS

Inchi: InChI=1S/C22H43N3O6/c1-17(2)14-29-20(26)23-10-7-8-12-25(22(28)31-16-19(5)6)13-9-
InchiKey: OGYFAOXNHYFWEE-UHFFFAOYSA-N
Formula: C22H43N3O6
SMILES: CC(C)COC(=O)NCCCCN(CCCNC(=O)OCC(C)C)C(=O)OCC(C)C
Mol. weight [g/mol]: 445.59

Physical Properties

Property code	Value	Unit	Source
gf	-285.16	kJ/mol	Joback Method
hf	-1073.18	kJ/mol	Joback Method
hfus	63.75	kJ/mol	Joback Method
hvap	105.78	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.016		Crippen Method
mcvol	373.100	ml/mol	McGowan Method
pc	1011.66	kPa	Joback Method
rinpol	3036.00		NIST Webbook
tb	1043.09	K	Joback Method
tc	1287.27	K	Joback Method
tf	646.97	K	Joback Method
vc	1.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1308.74	J/mol×K	1043.09	Joback Method
cpg	1323.96	J/mol×K	1083.79	Joback Method
cpg	1337.10	J/mol×K	1124.48	Joback Method
cpg	1348.22	J/mol×K	1165.18	Joback Method
cpg	1357.35	J/mol×K	1205.88	Joback Method
cpg	1364.56	J/mol×K	1246.58	Joback Method
cpg	1369.87	J/mol×K	1287.27	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R392840&Units=SI

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