Spermidine, tris-MOC derivative

Inchi: InChI=1S/C12H23N3O6/c1-19-10(16)13-6-4-8-15(12(18)21-3)9-5-7-14-11(17)20-2/h4-9H
InchiKey: XUDCEKFZZBVYFS-UHFFFAOYSA-N
Formula: C12H23N3O6
SMILES: COC(=O)NCCCN(CCCNC(=O)OC)C(=O)OC
Mol. weight [g/mol]: 305.33

Physical Properties

Property code	Value	Unit	Source
gf	-362.04	kJ/mol	Joback Method
hf	-850.94	kJ/mol	Joback Method
hfus	48.42	kJ/mol	Joback Method
hvap	84.69	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	0.547		Crippen Method
mcvol	232.200	ml/mol	McGowan Method
pc	2051.17	kPa	Joback Method
rinpol	2365.00		NIST Webbook
rinpol	2365.00		NIST Webbook
tb	815.61	K	Joback Method
tc	1007.77	K	Joback Method
tf	579.27	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	712.62	J/mol×K	815.61	Joback Method
cpg	725.28	J/mol×K	847.64	Joback Method
cpg	737.02	J/mol×K	879.66	Joback Method
cpg	747.82	J/mol×K	911.69	Joback Method
cpg	757.69	J/mol×K	943.71	Joback Method
cpg	766.63	J/mol×K	975.74	Joback Method
cpg	774.64	J/mol×K	1007.77	Joback Method

Sources

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=R333732&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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