N-[4-aminobutyl]-1,5-diaminopentane, tris-MOC derivative

Inchi: InChI=1S/C15H29N3O6/c1-22-13(19)16-9-5-4-7-11-18(15(21)24-3)12-8-6-10-17-14(20)2

InchiKey: JSWKTZMGYFVJBM-UHFFFAOYSA-N

Formula: C15H29N3O6

SMILES: COC(=O)NCCCCCN(CCCCNC(=O)OC)C(=O)OC

Mol. weight [g/mol]: 347.41

Physical Properties

Property code	Value	Unit	Source
gf	-336.78	kJ/mol	Joback Method
hf	-912.86	kJ/mol	Joback Method
hfus	56.19	kJ/mol	Joback Method
hvap	91.37	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	1.717		Crippen Method
mcvol	274.470	ml/mol	McGowan Method
pc	1605.13	kPa	Joback Method
rinpol	2570.00		NIST Webbook
tb	884.25	K	Joback Method
tc	1083.75	K	Joback Method
tf	613.08	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.98	J/mol×K	884.25	Joback Method
cpg	898.63	J/mol×K	917.50	Joback Method
cpg	911.13	J/mol×K	950.75	Joback Method
cpg	922.50	J/mol×K	984.00	Joback Method
cpg	932.73	J/mol×K	1017.25	Joback Method
cpg	941.83	J/mol×K	1050.50	Joback Method
cpg	949.82	J/mol×K	1083.75	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=R333707&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