N*1*-[4-(4-Amino-butylamino)-butyl]-butane-1,4-di tetrakis-MOC derivative

Inchi: InChI=1S/C20H38N4O8/c1-29-17(25)21-11-5-7-13-23(19(27)31-3)15-9-10-16-24(20(28)3
InchiKey: MUFKRSHAGSYVQG-UHFFFAOYSA-N
Formula: C20H38N4O8
SMILES: COC(=O)NCCCCN(CCCCN(CCCCNC(=O)OC)C(=O)OC)C(=O)OC
Mol. weight [g/mol]: 462.54

Physical Properties

Property code	Value	Unit	Source
gf	-417.82	kJ/mol	Joback Method
hf	-1193.33	kJ/mol	Joback Method
hfus	74.94	kJ/mol	Joback Method
hvap	113.70	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.176		Crippen Method
mcvol	362.340	ml/mol	McGowan Method
pc	1163.25	kPa	Joback Method
rinpol	3268.00		NIST Webbook
rinpol	3268.00		NIST Webbook
tb	1087.38	K	Joback Method
tc	1352.29	K	Joback Method
tf	774.06	K	Joback Method
vc	1.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1261.45	J/mol×K	1087.38	Joback Method
cpg	1273.01	J/mol×K	1131.53	Joback Method
cpg	1282.09	J/mol×K	1175.68	Joback Method
cpg	1288.71	J/mol×K	1219.83	Joback Method
cpg	1292.90	J/mol×K	1263.98	Joback Method
cpg	1294.70	J/mol×K	1308.14	Joback Method
cpg	1294.15	J/mol×K	1352.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R333678&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