N*1*-[3-(4-Amino-butylamino)-propyl]-butane-1,4-(tetrakis-MOC derivative

Inchi: InChI=1S/C19H36N4O8/c1-28-16(24)20-10-5-7-12-22(18(26)30-3)14-9-15-23(19(27)31-4

InchiKey: VXJCYSGKVUGEHN-UHFFFAOYSA-N

Formula: C19H36N4O8

SMILES: COC(=O)NCCCCN(CCCN(CCCCNC(=O)OC)C(=O)OC)C(=O)OC

Mol. weight [g/mol]: 448.51

Physical Properties

Property code	Value	Unit	Source
gf	-426.24	kJ/mol	Joback Method
hf	-1172.69	kJ/mol	Joback Method
hfus	72.35	kJ/mol	Joback Method
hvap	111.47	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	1.786		Crippen Method
mcvol	348.250	ml/mol	McGowan Method
pc	1243.33	kPa	Joback Method
rinpol	3162.00		NIST Webbook
rinpol	3162.00		NIST Webbook
tb	1064.50	K	Joback Method
tc	1317.44	K	Joback Method
tf	762.79	K	Joback Method
vc	1.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1201.53	J/mol×K	1064.50	Joback Method
cpg	1213.08	J/mol×K	1106.66	Joback Method
cpg	1222.39	J/mol×K	1148.81	Joback Method
cpg	1229.48	J/mol×K	1190.97	Joback Method
cpg	1234.39	J/mol×K	1233.13	Joback Method
cpg	1237.14	J/mol×K	1275.28	Joback Method
cpg	1237.74	J/mol×K	1317.44	Joback Method

Sources

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=R333663&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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