Nonanedioic acid, bis(8,8-dimethyl-2-oxabicyclo[4.2.0]octan-7-yl) ester

Inchi: InChI=1S/C27H44O6/c1-26(2)22-18(12-10-16-30-22)24(26)32-20(28)14-8-6-5-7-9-15-21(29)33-25-19-13-11-17-31-23(19)27(25,3)4/h18-19,22-25H,5-17H2,1-4H3/t18-,19-,22+,23+,24+,25+/m1/s1

InchiKey: BKZWWJZOYXKLFW-UHFFFAOYSA-N

Formula: C27H44O6

SMILES: CC1(C)C2OCCCC2C1OC(=O)CCCCCCCC(=O)OC1C2CCCOC2C1(C)C

Mol. weight [g/mol]: 464.63

CAS: 100996-43-8

Physical Properties

Property code	Value	Unit	Source
gf	-310.84	kJ/mol	Joback Method
hf	-1138.53	kJ/mol	Joback Method
hfus	63.05	kJ/mol	Joback Method
hvap	99.83	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	5.211		Crippen Method
mcvol	374.470	ml/mol	McGowan Method
pc	1002.71	kPa	Joback Method
tb	1049.48	K	Joback Method
tc	1285.69	K	Joback Method
tf	680.03	K	Joback Method
vc	1.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1474.00	J/mol×K	1049.48	Joback Method
cpg	1506.78	J/mol×K	1088.85	Joback Method
cpg	1540.57	J/mol×K	1128.22	Joback Method
cpg	1575.72	J/mol×K	1167.59	Joback Method
cpg	1612.56	J/mol×K	1206.95	Joback Method
cpg	1651.43	J/mol×K	1246.32	Joback Method
cpg	1692.68	J/mol×K	1285.69	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=C100996438&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume