Dimethyl carbocampesteryloxy glutarate

Inchi: InChI=1S/C36H59NO6/c1-22(2)23(3)9-10-24(4)28-13-14-29-27-12-11-25-21-26(17-19-35
InchiKey: AKBJDAPKDCGLBG-UHFFFAOYSA-N
Formula: C36H59NO6
SMILES: COC(=O)CCC(NC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)CCC(C)C(C)C)CCC32
Mol. weight [g/mol]: 601.86
CAS: 107928-38-1

Physical Properties

Property code	Value	Unit	Source
gf	-201.17	kJ/mol	Joback Method
hf	-1212.25	kJ/mol	Joback Method
hfus	61.85	kJ/mol	Joback Method
hvap	126.32	kJ/mol	Joback Method
log10ws	-9.13		Crippen Method
logp	7.863		Crippen Method
mcvol	502.660	ml/mol	McGowan Method
pc	680.29	kPa	Joback Method
tb	1339.28	K	Joback Method
tc	1678.39	K	Joback Method
tf	807.14	K	Joback Method
vc	1.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2212.76	J/mol×K	1339.28	Joback Method
cpg	2282.95	J/mol×K	1395.80	Joback Method
cpg	2359.50	J/mol×K	1452.32	Joback Method
cpg	2443.49	J/mol×K	1508.84	Joback Method
cpg	2535.95	J/mol×K	1565.35	Joback Method
cpg	2637.95	J/mol×K	1621.87	Joback Method
cpg	2750.54	J/mol×K	1678.39	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=C107928381&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume