Aldehyde of bryodulcosigenine 5

Inchi: InChI=1S/C27H42O3/c1-17(8-7-15-28)18-13-14-25(4)21-11-9-19-20(10-12-22(29)24(19,
InchiKey: CONXLKZYRPNXQH-UHFFFAOYSA-N
Formula: C27H42O3
SMILES: CC(CCC=O)C1CCC2(C)C3CC=C4C(CCC(O)C4(C)C)C3(C)C(=O)CC12C
Mol. weight [g/mol]: 414.62

Physical Properties

Property code	Value	Unit	Source
gf	-34.88	kJ/mol	Joback Method
hf	-695.09	kJ/mol	Joback Method
hfus	30.01	kJ/mol	Joback Method
hvap	98.58	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	5.747		Crippen Method
mcvol	352.560	ml/mol	McGowan Method
pc	1199.79	kPa	Joback Method
tb	1060.11	K	Joback Method
tc	1302.73	K	Joback Method
tf	696.17	K	Joback Method
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1436.53	J/mol×K	1060.11	Joback Method
cpg	1485.05	J/mol×K	1100.55	Joback Method
cpg	1537.76	J/mol×K	1140.98	Joback Method
cpg	1595.27	J/mol×K	1181.42	Joback Method
cpg	1658.16	J/mol×K	1221.86	Joback Method
cpg	1727.04	J/mol×K	1262.29	Joback Method
cpg	1802.51	J/mol×K	1302.73	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=B6009951&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

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