GA34, methyl ester

Inchi: InChI=1S/C20H26O6/c1-9-6-19-7-10(9)4-5-12(19)20-8-11(21)15(22)18(2,17(24)26-20)14
InchiKey: KWOJOQRTFRJBKX-BLYQCQJHSA-N
Formula: C20H26O6
SMILES: C=C1CC23CC1CCC2C12CC(O)C(O)C(C)(C(=O)O1)C2C3C(=O)OC
Mol. weight [g/mol]: 362.42

Physical Properties

Property code	Value	Unit	Source
gf	-313.43	kJ/mol	Joback Method
hf	-874.81	kJ/mol	Joback Method
hfus	36.71	kJ/mol	Joback Method
hvap	106.76	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	1.195		Crippen Method
mcvol	260.680	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
rinpol	2722.00		NIST Webbook
rinpol	2722.00		NIST Webbook
tb	1035.86	K	Joback Method
tc	1272.35	K	Joback Method
tf	754.83	K	Joback Method
vc	0.989	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.83	J/mol×K	1035.86	Joback Method
cpg	1097.47	J/mol×K	1075.27	Joback Method
cpg	1135.23	J/mol×K	1114.69	Joback Method
cpg	1176.56	J/mol×K	1154.10	Joback Method
cpg	1221.93	J/mol×K	1193.52	Joback Method
cpg	1271.78	J/mol×K	1232.93	Joback Method
cpg	1326.58	J/mol×K	1272.35	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=R565201&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