9,11-didehydro GA4

Inchi: InChI=1S/C20H24O5/c1-10-8-19-9-11(10)4-5-12(19)20-7-6-13(21)18(2,17(23)25-20)15(2
InchiKey: CSOGGDRRRLWUTQ-FNAXEMECSA-N
Formula: C20H24O5
SMILES: C=C1CC23CC1CC=C2C12CCC(O)C(C)(C(=O)O1)C2C3C(=O)OC
Mol. weight [g/mol]: 344.40

Physical Properties

Property code	Value	Unit	Source
gf	-140.86	kJ/mol	Joback Method
hf	-635.59	kJ/mol	Joback Method
hfus	31.32	kJ/mol	Joback Method
hvap	91.66	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	2.145		Crippen Method
mcvol	250.510	ml/mol	McGowan Method
pc	2133.46	kPa	Joback Method
rinpol	2494.00		NIST Webbook
rinpol	2492.00		NIST Webbook
rinpol	2492.00		NIST Webbook
tb	957.16	K	Joback Method
tc	1195.70	K	Joback Method
tf	715.77	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	935.80	J/mol×K	957.16	Joback Method
cpg	964.93	J/mol×K	996.92	Joback Method
cpg	996.55	J/mol×K	1036.67	Joback Method
cpg	1031.13	J/mol×K	1076.43	Joback Method
cpg	1069.16	J/mol×K	1116.19	Joback Method
cpg	1111.10	J/mol×K	1155.95	Joback Method
cpg	1157.46	J/mol×K	1195.70	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=R258394&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume