Desoxyadhumulone

Inchi: InChI=1S/C21H30O4/c1-7-14(6)18(22)17-20(24)15(10-8-12(2)3)19(23)16(21(17)25)11-9
InchiKey: VXESUOYBWMDWCJ-UHFFFAOYSA-N
Formula: C21H30O4
SMILES: CCC(C)C(=O)c1c(O)c(CC=C(C)C)c(O)c(CC=C(C)C)c1O
Mol. weight [g/mol]: 346.46

Physical Properties

Property code	Value	Unit	Source
gf	-232.79	kJ/mol	Joback Method
hf	-698.11	kJ/mol	Joback Method
hfus	56.62	kJ/mol	Joback Method
hvap	111.42	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	5.050		Crippen Method
mcvol	293.570	ml/mol	McGowan Method
pc	1888.72	kPa	Joback Method
rinpol	2365.00		NIST Webbook
rinpol	2364.00		NIST Webbook
tb	1019.89	K	Joback Method
tc	1258.44	K	Joback Method
tf	709.90	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	983.40	J/mol×K	1019.89	Joback Method
cpg	1004.24	J/mol×K	1059.65	Joback Method
cpg	1025.99	J/mol×K	1099.41	Joback Method
cpg	1048.94	J/mol×K	1139.17	Joback Method
cpg	1073.34	J/mol×K	1178.93	Joback Method
cpg	1099.45	J/mol×K	1218.68	Joback Method
cpg	1127.55	J/mol×K	1258.44	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=R97018&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume