Desoxycohumulone

Inchi:	InChI=1S/C20H28O4/c1-11(2)7-9-14-18(22)15(10-8-12(3)4)20(24)16(19(14)23)17(21)13
InchiKey:	KKFIZYKKQLWBKH-UHFFFAOYSA-N
Formula:	C20H28O4
SMILES:	CC(C)=CCc1c(O)c(CC=C(C)C)c(O)c(C(=O)C(C)C)c1O
Mol. weight [g/mol]:	332.43

Physical Properties

Property code	Value	Unit	Source
gf	-241.21	kJ/mol	Joback Method
hf	-677.47	kJ/mol	Joback Method
hfus	54.03	kJ/mol	Joback Method
hvap	109.19	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.660		Crippen Method
mcvol	279.480	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
rinpol	2317.00		NIST Webbook
rinpol	2317.00		NIST Webbook
tb	997.01	K	Joback Method
tc	1235.35	K	Joback Method
tf	698.63	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	920.20	J/mol×K	997.01	Joback Method
cpg	939.76	J/mol×K	1036.73	Joback Method
cpg	960.15	J/mol×K	1076.46	Joback Method
cpg	981.61	J/mol×K	1116.18	Joback Method
cpg	1004.42	J/mol×K	1155.91	Joback Method
cpg	1028.84	J/mol×K	1195.63	Joback Method
cpg	1055.11	J/mol×K	1235.35	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=R97036&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

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