2,6-Diacetyl-3,7,9-trihydroxy-8,9b-dimethyl-9bH-di (Usnic acid)

Inchi: InChI=1S/C18H16O7/c1-6-14(22)12(8(3)20)16-13(15(6)23)18(4)10(25-16)5-9(21)11(7(2)
InchiKey: WEYVVCKOOFYHRW-UHFFFAOYSA-N
Formula: C18H16O7
SMILES: CC(=O)C1=C(O)C=C2Oc3c(C(C)=O)c(O)c(C)c(O)c3C2(C)C1=O
Mol. weight [g/mol]: 344.32

Physical Properties

Property code	Value	Unit	Source
gf	-585.76	kJ/mol	Joback Method
hf	-958.27	kJ/mol	Joback Method
hfus	49.67	kJ/mol	Joback Method
hvap	126.61	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.127		Crippen Method
mcvol	238.590	ml/mol	McGowan Method
pc	3348.98	kPa	Joback Method
rinpol	2706.00		NIST Webbook
rinpol	2706.00		NIST Webbook
tb	1144.71	K	Joback Method
tc	1405.53	K	Joback Method
tf	935.09	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.72	J/mol×K	1144.71	Joback Method
cpg	877.12	J/mol×K	1188.18	Joback Method
cpg	908.43	J/mol×K	1231.65	Joback Method
cpg	943.01	J/mol×K	1275.12	Joback Method
cpg	981.23	J/mol×K	1318.59	Joback Method
cpg	1023.43	J/mol×K	1362.06	Joback Method
cpg	1069.97	J/mol×K	1405.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R627928&Units=SI
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

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