(+)-Usnic acid

Other names:	1,3(2H,9bH)-Dibenzofurandione, 2,6-diacetyl-7,9-dihydroxy-8,9b-dimethyl-, (9bR)- 3(9bH)-Dibenzofuranone, 2,6-diacetyl-1,7,9-trihydroxy-8,9b-dimethyl-, D- 3(9bH)-Dibenzofuranone, 2,6-diacetyl-8,9b-dimethyl-1,7,9-trihydroxy-, D- d-Usnic acid Usnic acid, (R)- (+)-Usninic acid d-Usninic acid 2,6-Diacetyl-7,9-dihydroxy-8,9b-dimethyldibenzo[b,d]furan-1,3(2H,9bh)-dione, (9bR)- (9bR)-2,6-diacetyl-7,9-dihydroxy-8,9b-dimethyl-(2H,9bH)-dibenzofuran-1,3-dione (9bR)-2,6-Diacetyl-7,9-dihydroxy-8,9b-dimethyldibenzo[b,d]furan-1,3(2H,9bH)-dione
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:	CUCUKLJLRRAKFN-UHFFFAOYSA-N
Formula:	C18H16O7
SMILES:	CC(=O)c1c(O)c(C)c(O)c2c1OC1=CC(=O)C(C(C)=O)C(=O)C12C
Mol. weight [g/mol]:	344.32
CAS:	7562-61-0

Physical Properties

Property code	Value	Unit	Source
gf	-589.94	kJ/mol	Joback Method
hf	-998.92	kJ/mol	Joback Method
hfus	45.72	kJ/mol	Joback Method
hvap	112.25	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	1.500		Crippen Method
mcvol	238.590	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
rinpol	2735.60		NIST Webbook
rinpol	2735.60		NIST Webbook
tb	1106.56	K	Joback Method
tc	1375.41	K	Joback Method
tf	912.45	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.37	J/mol×K	1106.56	Joback Method
cpg	873.37	J/mol×K	1151.37	Joback Method
cpg	900.44	J/mol×K	1196.18	Joback Method
cpg	929.89	J/mol×K	1240.99	Joback Method
cpg	962.07	J/mol×K	1285.79	Joback Method
cpg	997.29	J/mol×K	1330.60	Joback Method
cpg	1035.90	J/mol×K	1375.41	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7562610&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