

2',6'-Dihydroxyacetophenone, acetate

Inchi:	InChI=1S/C10H10O4/c1-6(11)10-8(13)4-3-5-9(10)14-7(2)12/h3-5,13H,1-2H3
InchiKey:	FYAUIMDHUAKCPA-UHFFFAOYSA-N
Formula:	C10H10O4
SMILES:	CC(=O)Oc1cccc(O)c1C(C)=O
Mol. weight [g/mol]:	194.18

Physical Properties

Property code	Value	Unit	Source
gf	-381.36	kJ/mol	Joback Method
hf	-559.36	kJ/mol	Joback Method
hfus	25.48	kJ/mol	Joback Method
hvap	69.71	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	1.520		Crippen Method
mvol	142.880	ml/mol	McGowan Method
pc	3886.79	kPa	Joback Method
rinpol	1502.40		NIST Webbook
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tb	670.64	K	Joback Method
tc	901.51	K	Joback Method
tf	475.21	K	Joback Method
vc	0.483	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.56	J/molxK	670.64	Joback Method
cpg	371.12	J/molxK	709.12	Joback Method
cpg	380.98	J/molxK	747.60	Joback Method
cpg	390.21	J/molxK	786.08	Joback Method
cpg	398.87	J/molxK	824.55	Joback Method
cpg	407.01	J/molxK	863.03	Joback Method
cpg	414.68	J/molxK	901.51	Joback Method
dvisc	0.0003480	Paxs	475.21	Joback Method

dvisc	0.0001932	Paxs	507.78	Joback Method
dvisc	0.0001151	Paxs	540.35	Joback Method
dvisc	0.0000727	Paxs	572.92	Joback Method
dvisc	0.0000483	Paxs	605.50	Joback Method
dvisc	0.0000334	Paxs	638.07	Joback Method
dvisc	0.0000240	Paxs	670.64	Joback Method

Sources

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=U352814&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_cvol:	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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