

jensenone

Inchi:	InChI=1S/C13H14O6/c1-6(2)3-9(16)10-12(18)7(4-14)11(17)8(5-15)13(10)19/h4-6,17-19H
InchiKey:	LGXKQDDWMRYQJK-UHFFFAOYSA-N
Formula:	C13H14O6
SMILES:	CC(C)CC(=O)c1c(O)c(C=O)c(O)c(C=O)c1O
Mol. weight [g/mol]:	266.25

Physical Properties

Property code	Value	Unit	Source
gf	-642.53	kJ/mol	Joback Method
hf	-919.01	kJ/mol	Joback Method
hfus	42.69	kJ/mol	Joback Method
hvap	106.97	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	1.657		Crippen Method
mvol	192.590	ml/mol	McGowan Method
pc	4450.38	kPa	Joback Method
rinpol	1839.00		NIST Webbook
rinpol	1839.00		NIST Webbook
tb	926.09	K	Joback Method
tc	1164.78	K	Joback Method
tf	741.82	K	Joback Method
vc	0.588	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.04	J/molxK	926.09	Joback Method
cpg	593.55	J/molxK	965.87	Joback Method
cpg	605.52	J/molxK	1005.65	Joback Method
cpg	618.12	J/molxK	1045.43	Joback Method
cpg	631.56	J/molxK	1085.21	Joback Method
cpg	646.01	J/molxK	1125.00	Joback Method
cpg	661.69	J/molxK	1164.78	Joback Method
dvisc	0.0000002	Paxs	741.82	Joback Method

dvisc	0.0000001	Paxs	772.53	Joback Method
dvisc	8.5812367e-08	Paxs	803.24	Joback Method
dvisc	5.5074177e-08	Paxs	833.95	Joback Method
dvisc	3.6477748e-08	Paxs	864.67	Joback Method
dvisc	2.4853182e-08	Paxs	895.38	Joback Method
dvisc	1.7369562e-08	Paxs	926.09	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=R301785&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	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:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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