2-Propen-1-one, 1-(2,6-dihydroxy-4-methoxyphenyl)-3-phenyl-

Other names: 2',6'-dihydroxy-4'-methoxychalcone
Inchi: InChI=1S/C16H14O4/c1-20-12-9-14(18)16(15(19)10-12)13(17)8-7-11-5-3-2-4-6-11/h2-10
InchiKey: CUGDOWNTXKLQMD-BQYQJAHWSA-N
Formula: C16H14O4
SMILES: COc1cc(O)c(C(=O)C=Cc2ccccc2)c(O)c1
Mol. weight [g/mol]: 270.28
CAS: 77129-49-8

Physical Properties

Property code	Value	Unit	Source
gf	-163.91	kJ/mol	Joback Method
hf	-394.18	kJ/mol	Joback Method
hfus	39.44	kJ/mol	Joback Method
hvap	91.57	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	3.002		Crippen Method
mcvol	203.660	ml/mol	McGowan Method
pc	3415.86	kPa	Joback Method
rinpol	2365.00		NIST Webbook
rinpol	2365.00		NIST Webbook
tb	865.51	K	Joback Method
tc	1120.65	K	Joback Method
tf	625.96	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	587.09	J/mol×K	865.51	Joback Method
cpg	649.86	J/mol×K	1078.13	Joback Method
cpg	636.96	J/mol×K	1035.60	Joback Method
cpg	624.45	J/mol×K	993.08	Joback Method
cpg	612.11	J/mol×K	950.56	Joback Method
cpg	599.73	J/mol×K	908.03	Joback Method

cpg	663.34	J/mol×K	1120.65	Joback Method
dvisc	0.0000003	Pa×s	865.51	Joback Method
dvisc	0.0000004	Pa×s	825.59	Joback Method
dvisc	0.0000006	Pa×s	785.66	Joback Method
dvisc	0.0000010	Pa×s	745.74	Joback Method
dvisc	0.0000016	Pa×s	705.81	Joback Method
dvisc	0.0000030	Pa×s	665.88	Joback Method
dvisc	0.0000060	Pa×s	625.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77129498&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
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
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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