Xanthoxylin

Other names:	Ethanone, 1-(2-hydroxy-4,6-dimethoxyphenyl)-
	Acetophenone, 2'-hydroxy-4',6'-dimethoxy-
	Brevifolin
	Brevifolin (Zanthoxylum)
	Phloracetophenone dimethyl ether
	Phloroacetophenone 2,4-dimethyl ether
	2-Hydroxy-4,6-dimethoxyacetophenone
	2,4-Di-O-methylphloroacetophenone
	2'-Hydroxy-4',6'-dimethoxyacetophenone
	4,6-Dimethoxy-2-hydroxyacetophenone
	1-Acetyl-2-hydroxy-4,6-dimethoxybenzene
	2-Hydroxyl-4,6-dimethoxy-acetophenone
	2-Acetyl-3,5-dimethoxyphenol
	NSC 17392
	Phloroacetophenone, dimethyl ether
	1-(2-hydroxy-4,6-dimethoxyphenyl)ethan-1-one
Inchi:	InChI=1S/C10H12O4/c1-6(11)10-8(12)4-7(13-2)5-9(10)14-3/h4-5,12H,1-3H3
InchiKey:	FBUBVLUPUDBFME-UHFFFAOYSA-N
Formula:	C10H12O4
SMILES:	COc1cc(O)c(C(C)=O)c(OC)c1
Mol. weight [g/mol]:	196.20
CAS:	90-24-4

Physical Properties

Property code	Value	Unit	Source
gf	-367.07	kJ/mol	Joback Method
hf	-590.47	kJ/mol	Joback Method
hfus	24.68	kJ/mol	Joback Method
hvap	66.03	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.612		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
rinpol	1667.00		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1675.20		NIST Webbook

rinpol	1625.00		NIST Webbook
rinpol	1675.20		NIST Webbook
tb	644.17	K	Joback Method
tc	866.56	K	Joback Method
tf	460.03	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.54	J/mol×K	644.17	Joback Method
cpg	423.15	J/mol×K	829.49	Joback Method
cpg	413.99	J/mol×K	792.43	Joback Method
cpg	404.28	J/mol×K	755.36	Joback Method
cpg	393.99	J/mol×K	718.30	Joback Method
cpg	383.08	J/mol×K	681.23	Joback Method
cpg	431.80	J/mol×K	866.56	Joback Method
dvisc	0.0000209	Pa×s	644.17	Joback Method
dvisc	0.0000290	Pa×s	613.48	Joback Method
dvisc	0.0000415	Pa×s	582.79	Joback Method
dvisc	0.0000619	Pa×s	552.10	Joback Method
dvisc	0.0000967	Pa×s	521.41	Joback Method
dvisc	0.0001598	Pa×s	490.72	Joback Method
dvisc	0.0002824	Pa×s	460.03	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C90244&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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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