2-methoxy-4-(4-methyl-1,3-dioxolan-2-yl)phenol

Other names: Vanillin 1,2-propylene glycol acetal
Inchi: InChI=1S/C11H14O4/c1-7-6-14-11(15-7)8-3-4-9(12)10(5-8)13-2/h3-5,7,11-12H,6H2,1-2H
InchiKey: RFGCVZIIIHRESZ-UHFFFAOYSA-N
Formula: C11H14O4
SMILES: COc1cc(C2OCC(C)O2)ccc1O
Mol. weight [g/mol]: 210.23
CAS: 68527-74-2

Physical Properties

Property code	Value	Unit	Source
gf	-258.50	kJ/mol	Joback Method
hf	-578.70	kJ/mol	Joback Method
hfus	35.83	kJ/mol	Joback Method
hvap	67.41	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.835		Crippen Method
mcvol	154.710	ml/mol	McGowan Method
pc	3472.45	kPa	Joback Method
rinpol	1685.60		NIST Webbook
rinpol	1685.60		NIST Webbook
tb	650.29	K	Joback Method
tc	888.93	K	Joback Method
tf	446.42	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.90	J/mol×K	650.29	Joback Method
cpg	446.19	J/mol×K	690.06	Joback Method
cpg	460.43	J/mol×K	729.84	Joback Method
cpg	473.70	J/mol×K	769.61	Joback Method
cpg	486.07	J/mol×K	809.38	Joback Method
cpg	497.62	J/mol×K	849.16	Joback Method

cpg	508.41	J/mol×K	888.93	Joback Method
dvisc	0.0005967	Pa×s	446.42	Joback Method
dvisc	0.0003126	Pa×s	480.40	Joback Method
dvisc	0.0001784	Pa×s	514.38	Joback Method
dvisc	0.0001091	Pa×s	548.36	Joback Method
dvisc	0.0000707	Pa×s	582.33	Joback Method
dvisc	0.0000480	Pa×s	616.31	Joback Method
dvisc	0.0000340	Pa×s	650.29	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C68527742&Units=SI

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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