2-Propen-1-ol, 3-(4-hydroxy-3,5-dimethoxyphenyl), (E)-

Inchi: InChI=1S/C11H14O4/c1-14-9-6-8(4-3-5-12)7-10(15-2)11(9)13/h3-4,6-7,12-13H,5H2,1-2H

InchiKey: LZFOPEXOUVTGJS-ONEGZZNKSA-N

Formula: C11H14O4

SMILES: COc1cc(C=CCO)cc(OC)c1O

Mol. weight [g/mol]: 210.23

CAS: 20675-96-1

Physical Properties

Property code	Value	Unit	Source
gf	-286.33	kJ/mol	Joback Method
hf	-533.54	kJ/mol	Joback Method
hfus	29.96	kJ/mol	Joback Method
hvap	78.15	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.415		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
rinpol	2034.20		NIST Webbook
rinpol	1928.00		NIST Webbook
rinpol	2034.20		NIST Webbook
rinpol	1928.00		NIST Webbook
tb	709.52	K	Joback Method
tc	915.43	K	Joback Method
tf	477.11	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.49	J/mol×K	709.52	Joback Method
cpg	444.15	J/mol×K	743.84	Joback Method
cpg	454.28	J/mol×K	778.16	Joback Method
cpg	463.91	J/mol×K	812.47	Joback Method
cpg	473.10	J/mol×K	846.79	Joback Method

cpg	481.87	J/mol×K	881.11	Joback Method
cpg	490.29	J/mol×K	915.43	Joback Method
dvisc	0.0001414	Pa×s	477.11	Joback Method
dvisc	0.0000574	Pa×s	515.85	Joback Method
dvisc	0.0000264	Pa×s	554.58	Joback Method
dvisc	0.0000135	Pa×s	593.32	Joback Method
dvisc	0.0000074	Pa×s	632.05	Joback Method
dvisc	0.0000044	Pa×s	670.78	Joback Method
dvisc	0.0000028	Pa×s	709.52	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=C20675961&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