Stiripentol

Other names:	1-Penten-3-ol, 1-(1,3-benzodioxol-5-yl)-4,4-dimethyl-
	1-Penten-3-ol, 4,4-dimethyl-1-(3,4-methylenedioxyphenyl)-
	BCX 2600
	4,4-Dimethyl-1-(3,4-methylenedioxyphenyl)-1-penten-3-ol
	E(+) 4,4-dimethyl-1-(3,4-methylenedioxyphenyl)-1-penten-3-ol (stiripentol)
Inchi:	InChI=1S/C14H18O3/c1-14(2,3)13(15)7-5-10-4-6-11-12(8-10)17-9-16-11/h4-8,13,15H,9H
InchiKey:	IBLNKMRFIPWSOY-FNORWQNLSA-N
Formula:	C14H18O3
SMILES:	CC(C)(C)C(O)C=Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]:	234.29
CAS:	49763-96-4

Physical Properties

Property code	Value	Unit	Source
gf	0.17	kJ/mol	Joback Method
hf	-338.60	kJ/mol	Joback Method
hfus	31.65	kJ/mol	Joback Method
hvap	74.55	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	2.836		Crippen Method
mcvol	186.810	ml/mol	McGowan Method
pc	2643.39	kPa	Joback Method
tb	714.34	K	Joback Method
tc	929.69	K	Joback Method
tf	417.48	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.59	J/mol×K	929.69	Joback Method
cpg	590.60	J/mol×K	893.80	Joback Method
cpg	580.14	J/mol×K	857.91	Joback Method
cpg	569.11	J/mol×K	822.02	Joback Method

cpg	557.42	J/mol×K	786.12	Joback Method
cpg	544.95	J/mol×K	750.23	Joback Method
cpg	531.61	J/mol×K	714.34	Joback Method
dvisc	0.0022109	Pa×s	417.48	Joback Method
dvisc	0.0000545	Pa×s	714.34	Joback Method
dvisc	0.0000803	Pa×s	664.86	Joback Method
dvisc	0.0001260	Pa×s	615.39	Joback Method
dvisc	0.0002137	Pa×s	565.91	Joback Method
dvisc	0.0004011	Pa×s	516.43	Joback Method
dvisc	0.0008602	Pa×s	466.96	Joback Method
hfust	29.00	kJ/mol	348.20	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C49763964&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
hfust: Enthalpy of fusion at a given temperature
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume