

Dihydroconiferol

Other names:	guaiacyl propanol 3-(4-hydroxy-3-methoxyphenyl)-propan-1-ol 3-(4-guaiacyl)propanol 3-(4-hydroxy-3-methoxy-phenyl)-1-propanol 1-Propanol, 3-(4-hydroxy-3-methoxyphenyl)
Inchi:	InChI=1S/C10H14O3/c1-13-10-7-8(3-2-6-11)4-5-9(10)12/h4-5,7,11-12H,2-3,6H2,1H3
InchiKey:	MWOMNLDJNQWJMK-UHFFFAOYSA-N
Formula:	C10H14O3
SMILES:	COc1cc(CCCO)ccc1O
Mol. weight [g/mol]:	182.22

Physical Properties

Property code	Value	Unit	Source
hf	-442.39	kJ/mol	Cheméo Relay (1.0)
hfus	26.37	kJ/mol	Joback Method
hvap	101.10	kJ/mol	Cheméo Relay (1.0)
ie	8.24	eV	Cheméo Relay (1.0)
log10ws	-1.27		Cheméo Relay (1.0)
logp	1.326		Crippen Method
mcvol	145.610	ml/mol	McGowan Method
rinpol	1660.60		NIST Webbook
rinpol	1597.00		NIST Webbook
rinpol	1660.60		NIST Webbook
ripol	2969.00		NIST Webbook
ripol	2969.00		NIST Webbook
ripol	2970.00		NIST Webbook
ripol	2941.00		NIST Webbook
ripol	2970.00		NIST Webbook
ripol	2970.00		NIST Webbook
ripol	2980.00		NIST Webbook
ripol	2941.00		NIST Webbook
ripol	2980.00		NIST Webbook
ripol	2980.00		NIST Webbook
tb	590.05	K	Cheméo Relay (1.0)
tf	338.95	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.34	J/mol×K	655.08	Joback Method
cpg	395.11	J/mol×K	688.76	Joback Method
cpg	405.31	J/mol×K	722.45	Joback Method
cpg	414.98	J/mol×K	756.13	Joback Method
cpg	424.16	J/mol×K	789.81	Joback Method
cpg	432.90	J/mol×K	823.50	Joback Method
cpg	441.25	J/mol×K	857.18	Joback Method
dvisc	0.0004872	Pa×s	436.17	Joback Method
dvisc	0.0001812	Pa×s	472.66	Joback Method
dvisc	0.0000777	Pa×s	509.14	Joback Method
dvisc	0.0000373	Pa×s	545.62	Joback Method
dvisc	0.0000196	Pa×s	582.11	Joback Method
dvisc	0.0000111	Pa×s	618.60	Joback Method
dvisc	0.0000067	Pa×s	655.08	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2305137&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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