

Olivetol, dimethyl ether

Other names:	Benzene, 1,3-dimethoxy-5-pentyl
Inchi:	InChI=1S/C13H20O2/c1-4-5-6-7-11-8-12(14-2)10-13(9-11)15-3/h8-10H,4-7H2,1-3H3
InchiKey:	LSPSEUBXQFHRGA-UHFFFAOYSA-N
Formula:	C13H20O2
SMILES:	CCCCCc1cc(OC)cc(OC)c1
Mol. weight [g/mol]:	208.30

Physical Properties

Property code	Value	Unit	Source
gf	-58.27	kJ/mol	Joback Method
hf	-362.50	kJ/mol	Joback Method
hfus	25.07	kJ/mol	Joback Method
hvap	52.95	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.436		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
rinpol	1627.00		NIST Webbook
rinpol	1627.00		NIST Webbook
rinpol	1643.50		NIST Webbook
rinpol	1643.50		NIST Webbook
tb	578.32	K	Joback Method
tc	773.80	K	Joback Method
tf	332.19	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.62	J/mol×K	578.32	Joback Method
cpg	463.86	J/mol×K	610.90	Joback Method
cpg	479.37	J/mol×K	643.48	Joback Method
cpg	494.16	J/mol×K	676.06	Joback Method
cpg	508.24	J/mol×K	708.64	Joback Method

cpg	521.59	J/mol×K	741.22	Joback Method
cpg	534.23	J/mol×K	773.80	Joback Method
dvisc	0.0011010	Pa×s	332.19	Joback Method
dvisc	0.0006253	Pa×s	373.21	Joback Method
dvisc	0.0003973	Pa×s	414.23	Joback Method
dvisc	0.0002739	Pa×s	455.25	Joback Method
dvisc	0.0002008	Pa×s	496.28	Joback Method
dvisc	0.0001544	Pa×s	537.30	Joback Method
dvisc	0.0001232	Pa×s	578.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333367&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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