

3,6-Dimethoxy-4-phenanthrol

Other names:	4-O-Thebaol
Inchi:	InChI=1S/C16H14O3/c1-18-12-7-5-10-3-4-11-6-8-14(19-2)16(17)15(11)13(10)9-12/h3-9,
InchiKey:	GKDSKCYMUUXQLA-UHFFFAOYSA-N
Formula:	C16H14O3
SMILES:	COc1ccc2ccc3ccc(OC)c(O)c3c2c1
Mol. weight [g/mol]:	254.28
CAS:	481-81-2

Physical Properties

Property code	Value	Unit	Source
gf	16.04	kJ/mol	Joback Method
hf	-231.06	kJ/mol	Joback Method
hfus	32.27	kJ/mol	Joback Method
hvap	76.59	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	3.716		Crippen Method
mcvol	191.230	ml/mol	McGowan Method
pc	2881.21	kPa	Joback Method
rinpol	2522.00		NIST Webbook
rinpol	2522.00		NIST Webbook
tb	770.52	K	Joback Method
tc	1014.39	K	Joback Method
tf	555.64	K	Joback Method
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.31	J/molxK	770.52	Joback Method
cpg	587.99	J/molxK	973.74	Joback Method
cpg	576.97	J/molxK	933.10	Joback Method
cpg	565.62	J/molxK	892.45	Joback Method
cpg	553.82	J/molxK	851.81	Joback Method
cpg	541.42	J/molxK	811.16	Joback Method

cpg	598.80	J/mol×K	1014.39	Joback Method
dvisc	0.0000223	Paxs	770.52	Joback Method
dvisc	0.0000285	Paxs	734.71	Joback Method
dvisc	0.0000373	Paxs	698.89	Joback Method
dvisc	0.0000502	Paxs	663.08	Joback Method
dvisc	0.0000701	Paxs	627.27	Joback Method
dvisc	0.0001017	Paxs	591.45	Joback Method
dvisc	0.0001548	Paxs	555.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C481812&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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