

Benzene, 1,3-dimethoxy-4-hexyl-2-methyl

Inchi:	InChI=1S/C15H24O2/c1-5-6-7-8-9-13-10-11-14(16-3)12(2)15(13)17-4/h10-11H,5-9H2,1-
InchiKey:	SAMCUYQALYTYKN-UHFFFAOYSA-N
Formula:	C15H24O2
SMILES:	CCCCCc1ccc(OC)c(C)c1OC
Mol. weight [g/mol]:	236.35

Physical Properties

Property code	Value	Unit	Source
gf	-51.06	kJ/mol	Joback Method
hf	-415.25	kJ/mol	Joback Method
hfus	29.86	kJ/mol	Joback Method
hvap	58.07	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.135		Crippen Method
mvol	210.190	ml/mol	McGowan Method
pc	1727.46	kPa	Joback Method
rinpol	1718.00		NIST Webbook
rinpol	1718.00		NIST Webbook
tb	629.06	K	Joback Method
tc	820.74	K	Joback Method
tf	367.25	K	Joback Method
vc	0.803	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.38	J/molxK	629.06	Joback Method
cpg	567.61	J/molxK	661.01	Joback Method
cpg	584.06	J/molxK	692.95	Joback Method
cpg	599.72	J/molxK	724.90	Joback Method
cpg	614.61	J/molxK	756.85	Joback Method
cpg	628.72	J/molxK	788.80	Joback Method
cpg	642.05	J/molxK	820.74	Joback Method
dvisc	0.0008191	Paxs	367.25	Joback Method

dvisc	0.0004802	Paxs	410.88	Joback Method
dvisc	0.0003119	Paxs	454.52	Joback Method
dvisc	0.0002185	Paxs	498.15	Joback Method
dvisc	0.0001621	Paxs	541.79	Joback Method
dvisc	0.0001257	Paxs	585.42	Joback Method
dvisc	0.0001010	Paxs	629.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R143069&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
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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