

Benzene, 1,3-dimethoxy-4-heptyl

Inchi:	InChI=1S/C15H24O2/c1-4-5-6-7-8-9-13-10-11-14(16-2)12-15(13)17-3/h10-12H,4-9H2,1-
InchiKey:	FQMKORGESTUPOF-UHFFFAOYSA-N
Formula:	C15H24O2
SMILES:	CCCCCCCc1ccc(OC)cc1OC
Mol. weight [g/mol]:	236.35

Physical Properties

Property code	Value	Unit	Source
gf	-41.43	kJ/mol	Joback Method
hf	-403.78	kJ/mol	Joback Method
hfus	30.25	kJ/mol	Joback Method
hvap	57.40	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	4.217		Crippen Method
mcvol	210.190	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinqol	1782.00		NIST Webbook
tb	624.08	K	Joback Method
tc	814.87	K	Joback Method
tf	354.73	K	Joback Method
vc	0.803	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.39	J/molxK	624.08	Joback Method
cpg	567.80	J/molxK	655.88	Joback Method
cpg	584.39	J/molxK	687.68	Joback Method
cpg	600.18	J/molxK	719.47	Joback Method
cpg	615.17	J/molxK	751.27	Joback Method
cpg	629.37	J/molxK	783.07	Joback Method
cpg	642.78	J/molxK	814.87	Joback Method
dvisc	0.0010288	Paxs	354.73	Joback Method
dvisc	0.0005640	Paxs	399.62	Joback Method

dvisc	0.0003492	Paxs	444.51	Joback Method
dvisc	0.0002360	Paxs	489.41	Joback Method
dvisc	0.0001704	Paxs	534.30	Joback Method
dvisc	0.0001294	Paxs	579.19	Joback Method
dvisc	0.0001022	Paxs	624.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R143034&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
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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