Benzene, 1,3-dimethoxy-5-heptyl

Inchi: InChI=1S/C15H24O2/c1-4-5-6-7-8-9-13-10-14(16-2)12-15(11-13)17-3/h10-12H,4-9H2,1-3

InchiKey: RFHLFJVSZNEBHT-UHFFFAOYSA-N

Formula: C15H24O2

SMILES: CCCCCCCc1cc(OC)cc(OC)c1

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
rinpol	1830.00		NIST Webbook
rinpol	1830.00		NIST Webbook
tb	624.08	K	Joback Method
tc	814.87	K	Joback Method
tf	354.73	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.39	J/mol×K	624.08	Joback Method
cpg	629.37	J/mol×K	783.07	Joback Method
cpg	615.17	J/mol×K	751.27	Joback Method
cpg	600.18	J/mol×K	719.47	Joback Method
cpg	584.39	J/mol×K	687.68	Joback Method
cpg	567.80	J/mol×K	655.88	Joback Method
cpg	642.78	J/mol×K	814.87	Joback Method
dvisc	0.0001022	Pa×s	624.08	Joback Method

dvisc	0.0001294	Pa×s	579.19	Joback Method
dvisc	0.0001704	Pa×s	534.30	Joback Method
dvisc	0.0002360	Pa×s	489.41	Joback Method
dvisc	0.0003492	Pa×s	444.51	Joback Method
dvisc	0.0005640	Pa×s	399.62	Joback Method
dvisc	0.0010288	Pa×s	354.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R143163&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