

Benzene, 1,3-dimethoxy-5-methyl-2-octyl

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C17H28O2/c1-5-6-7-8-9-10-11-15-16(18-3)12-14(2)13-17(15)19-4/h12-13H,5-

AKFKVAMWKLBDN-UHFFFAOYSA-N

C17H28O2

CCCCCCCCc1c(OC)cc(C)cc1OC

264.40

Physical Properties

Property code	Value	Unit	Source
gf	-34.22	kJ/mol	Joback Method
hf	-456.53	kJ/mol	Joback Method
hfus	35.04	kJ/mol	Joback Method
hvap	62.52	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	4.915		Crippen Method
mcvol	238.370	ml/mol	McGowan Method
pc	1481.57	kPa	Joback Method
rinpol	1884.00		NIST Webbook
tb	674.82	K	Joback Method
tc	862.96	K	Joback Method
tf	389.79	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.98	J/mol×K	674.82	Joback Method
cpg	677.12	J/mol×K	706.18	Joback Method
cpg	694.38	J/mol×K	737.53	Joback Method
cpg	710.79	J/mol×K	768.89	Joback Method
cpg	726.34	J/mol×K	800.24	Joback Method
cpg	741.04	J/mol×K	831.60	Joback Method
cpg	754.90	J/mol×K	862.96	Joback Method
dvisc	0.0007460	Pa×s	389.79	Joback Method
dvisc	0.0004231	Pa×s	437.30	Joback Method

dvisc	0.0002682	Pa×s	484.80	Joback Method
dvisc	0.0001844	Pa×s	532.30	Joback Method
dvisc	0.0001348	Pa×s	579.81	Joback Method
dvisc	0.0001033	Pa×s	627.31	Joback Method
dvisc	0.0000822	Pa×s	674.82	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R143198&Units=SI

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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