

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

Inchi:	InChI=1S/C18H30O2/c1-5-6-7-8-9-10-11-12-16-17(19-3)13-15(2)14-18(16)20-4/h13-14H
InchiKey:	UEUWVQBOJBXOFO-UHFFFAOYSA-N
Formula:	C18H30O2
SMILES:	CCCCCCCCc1c(OC)cc(C)cc1OC
Mol. weight [g/mol]:	278.43

Physical Properties

Property code	Value	Unit	Source
gf	-25.80	kJ/mol	Joback Method
hf	-477.17	kJ/mol	Joback Method
hfus	37.63	kJ/mol	Joback Method
hvap	64.74	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.305		Crippen Method
mvol	252.460	ml/mol	McGowan Method
pc	1377.86	kPa	Joback Method
rinpol	1982.00		NIST Webbook
rinpol	1982.00		NIST Webbook
tb	697.70	K	Joback Method
tc	884.64	K	Joback Method
tf	401.06	K	Joback Method
vc	0.972	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.23	J/molxK	697.70	Joback Method
cpg	798.74	J/molxK	853.48	Joback Method
cpg	783.82	J/molxK	822.33	Joback Method
cpg	768.02	J/molxK	791.17	Joback Method
cpg	751.32	J/molxK	760.01	Joback Method
cpg	733.73	J/molxK	728.86	Joback Method
cpg	812.79	J/molxK	884.64	Joback Method
dvisc	0.0000736	Paxs	697.70	Joback Method

dvisc	0.0000929	Paxs	648.26	Joback Method
dvisc	0.0001218	Paxs	598.82	Joback Method
dvisc	0.0001677	Paxs	549.38	Joback Method
dvisc	0.0002460	Paxs	499.94	Joback Method
dvisc	0.0003926	Paxs	450.50	Joback Method
dvisc	0.0007031	Paxs	401.06	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R143183&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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