Benzene, 1,3-dimethoxy-2-nonyl

Inchi: InChI=1S/C17H28O2/c1-4-5-6-7-8-9-10-12-15-16(18-2)13-11-14-17(15)19-3/h11,13-14H
InchiKey: VFVMVMNLTQHDCD-UHFFFAOYSA-N
Formula: C17H28O2
SMILES: CCCCCCCCCc1c(OC)cccc1OC
Mol. weight [g/mol]: 264.40

Physical Properties

Property code	Value	Unit	Source
gf	-24.59	kJ/mol	Joback Method
hf	-445.06	kJ/mol	Joback Method
hfus	35.42	kJ/mol	Joback Method
hvap	61.86	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.997		Crippen Method
mcvol	238.370	ml/mol	McGowan Method
pc	1498.83	kPa	Joback Method
rinpol	1909.00		NIST Webbook
rinpol	1909.00		NIST Webbook
tb	669.84	K	Joback Method
tc	857.12	K	Joback Method
tf	377.27	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.97	J/mol×K	669.84	Joback Method
cpg	741.55	J/mol×K	825.91	Joback Method
cpg	726.77	J/mol×K	794.69	Joback Method
cpg	711.13	J/mol×K	763.48	Joback Method
cpg	694.63	J/mol×K	732.27	Joback Method
cpg	677.24	J/mol×K	701.05	Joback Method
cpg	755.49	J/mol×K	857.12	Joback Method
dvisc	0.0000826	Pa×s	669.84	Joback Method

dvisc	0.0001055	Pa×s	621.08	Joback Method
dvisc	0.0001405	Pa×s	572.32	Joback Method
dvisc	0.0001973	Pa×s	523.56	Joback Method
dvisc	0.0002971	Pa×s	474.79	Joback Method
dvisc	0.0004912	Pa×s	426.03	Joback Method
dvisc	0.0009250	Pa×s	377.27	Joback Method

Sources

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=R142917&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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