Benzene, 1,3-dimethoxy-4-heptyl-2-methyl

Inchi: InChI=1S/C16H26O2/c1-5-6-7-8-9-10-14-11-12-15(17-3)13(2)16(14)18-4/h11-12H,5-10H
InchiKey: MSXNMBAGZAFKKN-UHFFFAOYSA-N
Formula: C16H26O2
SMILES: CCCCCCCc1ccc(OC)c(C)c1OC
Mol. weight [g/mol]: 250.38

Physical Properties

Property code	Value	Unit	Source
gf	-42.64	kJ/mol	Joback Method
hf	-435.89	kJ/mol	Joback Method
hfus	32.45	kJ/mol	Joback Method
hvap	60.29	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.525		Crippen Method
mcvol	224.280	ml/mol	McGowan Method
pc	1597.44	kPa	Joback Method
rinpol	1812.00		NIST Webbook
rinpol	1812.00		NIST Webbook
tb	651.94	K	Joback Method
tc	841.67	K	Joback Method
tf	378.52	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.00	J/mol×K	651.94	Joback Method
cpg	684.35	J/mol×K	810.05	Joback Method
cpg	669.92	J/mol×K	778.43	Joback Method
cpg	654.67	J/mol×K	746.81	Joback Method
cpg	638.60	J/mol×K	715.18	Joback Method
cpg	621.71	J/mol×K	683.56	Joback Method
cpg	697.97	J/mol×K	841.67	Joback Method
dvisc	0.0000914	Pa×s	651.94	Joback Method

dvisc	0.0001143	Pa×s	606.37	Joback Method
dvisc	0.0001483	Pa×s	560.80	Joback Method
dvisc	0.0002014	Pa×s	515.23	Joback Method
dvisc	0.0002903	Pa×s	469.66	Joback Method
dvisc	0.0004526	Pa×s	424.09	Joback Method
dvisc	0.0007852	Pa×s	378.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R143049&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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