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

Inchi: InChI=1S/C11H16O2/c1-5-9-10(12-3)6-8(2)7-11(9)13-4/h6-7H,5H2,1-4H3
InchiKey: KBHCITMKIJKTSU-UHFFFAOYSA-N
Formula: C11H16O2
SMILES: CCc1c(OC)cc(C)cc1OC
Mol. weight [g/mol]: 180.24

Physical Properties

Property code	Value	Unit	Source
gf	-84.74	kJ/mol	Joback Method
hf	-332.69	kJ/mol	Joback Method
hfus	19.50	kJ/mol	Joback Method
hvap	49.16	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.575		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
pc	2445.89	kPa	Joback Method
rinpol	1348.00		NIST Webbook
tb	537.54	K	Joback Method
tc	739.59	K	Joback Method
tf	322.17	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.53	J/mol×K	537.54	Joback Method
cpg	365.89	J/mol×K	571.22	Joback Method
cpg	379.69	J/mol×K	604.89	Joback Method
cpg	392.91	J/mol×K	638.57	Joback Method
cpg	405.54	J/mol×K	672.24	Joback Method
cpg	417.58	J/mol×K	705.92	Joback Method
cpg	429.03	J/mol×K	739.59	Joback Method
dvisc	0.0008693	Pa×s	322.17	Joback Method
dvisc	0.0005502	Pa×s	358.06	Joback Method

dvisc	0.0003785	Pa×s	393.96	Joback Method
dvisc	0.0002772	Pa×s	429.86	Joback Method
dvisc	0.0002130	Pa×s	465.75	Joback Method
dvisc	0.0001699	Pa×s	501.64	Joback Method
dvisc	0.0001397	Pa×s	537.54	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=R142828&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