2-Allyl-1,4-dimethoxy-3-methyl-benzene

Inchi: InChI=1S/C12H16O2/c1-5-6-10-9(2)11(13-3)7-8-12(10)14-4/h5,7-8H,1,6H2,2-4H3
InchiKey: QVZBRUBDHWOPIM-UHFFFAOYSA-N
Formula: C12H16O2
SMILES: C=CCc1c(OC)ccc(OC)c1C
Mol. weight [g/mol]: 192.25

Physical Properties

Property code	Value	Unit	Source
gf	11.52	kJ/mol	Joback Method
hf	-227.90	kJ/mol	Joback Method
hfus	20.81	kJ/mol	Joback Method
hvap	50.72	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.741		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
rinpol	1601.00		NIST Webbook
tb	557.10	K	Joback Method
tc	760.27	K	Joback Method
tf	331.68	K	Joback Method
vc	0.617	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.89	J/mol×K	557.10	Joback Method
cpg	393.51	J/mol×K	590.96	Joback Method
cpg	407.50	J/mol×K	624.82	Joback Method
cpg	420.85	J/mol×K	658.69	Joback Method
cpg	433.56	J/mol×K	692.55	Joback Method
cpg	445.63	J/mol×K	726.41	Joback Method
cpg	457.05	J/mol×K	760.27	Joback Method
dvisc	0.0008345	Pa×s	331.68	Joback Method
dvisc	0.0005269	Pa×s	369.25	Joback Method

dvisc	0.0003622	Pa×s	406.82	Joback Method
dvisc	0.0002652	Pa×s	444.39	Joback Method
dvisc	0.0002039	Pa×s	481.96	Joback Method
dvisc	0.0001628	Pa×s	519.53	Joback Method
dvisc	0.0001340	Pa×s	557.10	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=U187537&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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