

1-Allyl-2,4-dimethoxybenzene

Other names:	1-Allyl-2,4-dimethoxybenzene Benzene, 1-(2-propenyl)-2,4-dimethoxy
Inchi:	InChI=1S/C11H14O2/c1-4-5-9-6-7-10(12-2)8-11(9)13-3/h4,6-8H,1,5H2,2-3H3
InchiKey:	HZLYHZSHPUFYAR-UHFFFAOYSA-N
Formula:	C11H14O2
SMILES:	C=CCc1ccc(OC)cc1OC
Mol. weight [g/mol]:	178.23

Physical Properties

Property code	Value	Unit	Source
hfus	18.61	kJ/mol	Joback Method
hvap	67.61	kJ/mol	Cheméo Relay (1.0)
ie	7.78	eV	Cheméo Relay (1.0)
log10ws	-3.03		Cheméo Relay (1.0)
logp	2.432		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
rinpol	1322.00		NIST Webbook
tb	528.20	K	Cheméo Relay (1.0)
tf	268.72	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.58	J/mol×K	529.24	Joback Method
cpg	346.58	J/mol×K	563.43	Joback Method
cpg	359.96	J/mol×K	597.63	Joback Method
cpg	372.71	J/mol×K	631.82	Joback Method
cpg	384.84	J/mol×K	666.01	Joback Method
cpg	396.35	J/mol×K	700.21	Joback Method
cpg	407.24	J/mol×K	734.40	Joback Method
dvisc	0.0010599	Pa×s	307.89	Joback Method
dvisc	0.0006390	Pa×s	344.78	Joback Method
dvisc	0.0004248	Pa×s	381.67	Joback Method
dvisc	0.0003035	Pa×s	418.56	Joback Method

dvisc	0.0002290	Pa×s	455.46	Joback Method
dvisc	0.0001802	Pa×s	492.35	Joback Method
dvisc	0.0001466	Pa×s	529.24	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3698235&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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