

1-Methoxy-4-(2-methylpropenyl)benzene

Other names:	2-Methyl-3-(4-methoxyphenyl)-prop-2-ene
Inchi:	InChI=1S/C11H14O/c1-9(2)8-10-4-6-11(12-3)7-5-10/h4-8H,1-3H3
InchiKey:	QABCSPDGWHIRHC-UHFFFAOYSA-N
Formula:	C11H14O
SMILES:	<chem>COc1ccc(C=C(C)C)cc1</chem>
Mol. weight [g/mol]:	162.23

Physical Properties

Property code	Value	Unit	Source
gf	111.19	kJ/mol	Joback Method
hf	-70.10	kJ/mol	Joback Method
hfus	17.98	kJ/mol	Joback Method
hvap	45.47	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.118		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
rinpol	1325.00		NIST Webbook
tb	509.20	K	Joback Method
tc	724.36	K	Joback Method
tf	255.86	K	Joback Method
vc	0.542	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.38	J/mol×K	509.20	Joback Method
cpg	323.47	J/mol×K	545.06	Joback Method
cpg	337.73	J/mol×K	580.92	Joback Method
cpg	351.19	J/mol×K	616.78	Joback Method
cpg	363.86	J/mol×K	652.64	Joback Method
cpg	375.80	J/mol×K	688.50	Joback Method
cpg	387.02	J/mol×K	724.36	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=R418427&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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