

3-Methyl-2,3-dihydro-benzofuran

Other names:	2,3-Dihydro-3-methylbenzofuran
Inchi:	InChI=1S/C9H10O/c1-7-6-10-9-5-3-2-4-8(7)9/h2-5,7H,6H2,1H3
InchiKey:	YZDGROPVYQGZTK-UHFFFAOYSA-N
Formula:	C9H10O
SMILES:	CC1COc2ccccc21
Mol. weight [g/mol]:	134.18
CAS:	13524-73-7

Physical Properties

Property code	Value	Unit	Source
gf	102.31	kJ/mol	Joback Method
hf	-63.23	kJ/mol	Joback Method
hfus	18.83	kJ/mol	Joback Method
hvap	42.99	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	2.183		Crippen Method
mcvol	108.920	ml/mol	McGowan Method
pc	3695.46	kPa	Joback Method
ripol	1655.00		NIST Webbook
tb	470.67	K	Joback Method
tc	696.07	K	Joback Method
tf	274.64	K	Joback Method
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.43	J/mol×K	470.67	Joback Method
cpg	243.71	J/mol×K	508.24	Joback Method
cpg	256.99	J/mol×K	545.80	Joback Method
cpg	269.35	J/mol×K	583.37	Joback Method
cpg	280.83	J/mol×K	620.94	Joback Method
cpg	291.50	J/mol×K	658.50	Joback Method
cpg	301.42	J/mol×K	696.07	Joback Method

dvisc	0.0016500	Pa×s	274.64	Joback Method
dvisc	0.0011869	Pa×s	307.31	Joback Method
dvisc	0.0009095	Pa×s	339.98	Joback Method
dvisc	0.0007303	Pa×s	372.65	Joback Method
dvisc	0.0006075	Pa×s	405.33	Joback Method
dvisc	0.0005194	Pa×s	438.00	Joback Method
dvisc	0.0004539	Pa×s	470.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13524737&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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