

2-isobutoxy-3,4-dihydro-2H-pyran

Inchi:	InChI=1S/C9H16O2/c1-8(2)7-11-9-5-3-4-6-10-9/h4,6,8-9H,3,5,7H2,1-2H3
InchiKey:	WGSJOWWPBIGTI-UHFFFAOYSA-N
Formula:	C9H16O2
SMILES:	CC(C)COC1CCC=CO1
Mol. weight [g/mol]:	156.22

Physical Properties

Property code	Value	Unit	Source
gf	-114.25	kJ/mol	Joback Method
hf	-386.49	kJ/mol	Joback Method
hfus	17.77	kJ/mol	Joback Method
hvap	42.88	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.309		Crippen Method
mcvol	134.250	ml/mol	McGowan Method
pc	2893.62	kPa	Joback Method
rinsol	1030.00		NIST Webbook
tb	472.96	K	Joback Method
tc	677.00	K	Joback Method
tf	233.13	K	Joback Method
vc	0.491	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.55	J/molxK	472.96	Joback Method
cpg	316.33	J/molxK	506.97	Joback Method
cpg	332.32	J/molxK	540.97	Joback Method
cpg	347.53	J/molxK	574.98	Joback Method
cpg	361.96	J/molxK	608.99	Joback Method
cpg	375.63	J/molxK	643.00	Joback Method
cpg	388.56	J/molxK	677.00	Joback Method
dvisc	0.0071498	Paxs	233.13	Joback Method
dvisc	0.0026630	Paxs	273.10	Joback Method

dvisc	0.0012763	Paxs	313.07	Joback Method
dvisc	0.0007226	Paxs	353.04	Joback Method
dvisc	0.0004593	Paxs	393.02	Joback Method
dvisc	0.0003174	Paxs	432.99	Joback Method
dvisc	0.0002335	Paxs	472.96	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R132915&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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