

2-Isopropoxy-1,3-cyclohexadiene

Inchi:	InChI=1S/C9H14O/c1-8(2)10-9-6-4-3-5-7-9/h4,6-8H,3,5H2,1-2H3
InchiKey:	FMQGDKGEHUYQJR-UHFFFAOYSA-N
Formula:	C9H14O
SMILES:	CC(C)OC1=CCCC=C1
Mol. weight [g/mol]:	138.21
CAS:	98677-91-9

Physical Properties

Property code	Value	Unit	Source
gf	-0.09	kJ/mol	Joback Method
hf	-187.84	kJ/mol	Joback Method
hfus	9.55	kJ/mol	Joback Method
hvap	39.63	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.645		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
tb	454.82	K	Joback Method
tc	663.37	K	Joback Method
tf	224.08	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.66	J/molxK	454.82	Joback Method
cpg	268.97	J/molxK	489.58	Joback Method
cpg	283.53	J/molxK	524.34	Joback Method
cpg	297.36	J/molxK	559.10	Joback Method
cpg	310.46	J/molxK	593.86	Joback Method
cpg	322.86	J/molxK	628.61	Joback Method
cpg	334.57	J/molxK	663.37	Joback Method
dvisc	0.0052852	Paxs	224.08	Joback Method
dvisc	0.0020524	Paxs	262.54	Joback Method

dvisc	0.0010150	Paxs	300.99	Joback Method
dvisc	0.0005887	Paxs	339.45	Joback Method
dvisc	0.0003815	Paxs	377.91	Joback Method
dvisc	0.0002679	Paxs	416.36	Joback Method
dvisc	0.0001997	Paxs	454.82	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=C98677919&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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