

2,3-Dimethyl-5-hexen-2-ol

Inchi:	InChI=1S/C8H16O/c1-5-6-7(2)8(3,4)9/h5,7,9H,1,6H2,2-4H3
InchiKey:	GRCJVLMMUNHFVRD-UHFFFAOYSA-N
Formula:	C8H16O
SMILES:	C=CCC(C)C(C)(C)O
Mol. weight [g/mol]:	128.21

Physical Properties

Property code	Value	Unit	Source
gf	-32.10	kJ/mol	Joback Method
hf	-249.28	kJ/mol	Joback Method
hfus	8.35	kJ/mol	Joback Method
hvap	47.73	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	1.969		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
ripol	1451.00		NIST Webbook
ripol	1451.00		NIST Webbook
ripol	1451.00		NIST Webbook
ripol	1451.00		NIST Webbook
tb	467.63	K	Joback Method
tc	643.35	K	Joback Method
tf	226.40	K	Joback Method
vc	0.467	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.88	J/mol×K	467.63	Joback Method
cpg	288.18	J/mol×K	496.92	Joback Method
cpg	299.85	J/mol×K	526.20	Joback Method
cpg	310.92	J/mol×K	555.49	Joback Method
cpg	321.41	J/mol×K	584.78	Joback Method
cpg	331.36	J/mol×K	614.06	Joback Method

cpg	340.78	J/mol×K	643.35	Joback Method
dvisc	0.1631928	Paxs	226.40	Joback Method
dvisc	0.0221752	Paxs	266.61	Joback Method
dvisc	0.0050841	Paxs	306.81	Joback Method
dvisc	0.0016398	Paxs	347.01	Joback Method
dvisc	0.0006690	Paxs	387.22	Joback Method
dvisc	0.0003231	Paxs	427.42	Joback Method
dvisc	0.0001768	Paxs	467.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R302788&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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