

4-Penten-2-ol, 3-methyl-

Other names:	3-Methyl-4-penten-2-ol
Inchi:	InChI=1S/C6H12O/c1-4-5(2)6(3)7/h4-7H,1H2,2-3H3
InchiKey:	COIPQIFWUIDWLU-UHFFFAOYSA-N
Formula:	C6H12O
SMILES:	C=CC(C)C(C)O
Mol. weight [g/mol]:	100.16
CAS:	1569-59-1

Physical Properties

Property code	Value	Unit	Source
gf	-54.22	kJ/mol	Joback Method
hf	-204.53	kJ/mol	Joback Method
hfus	7.06	kJ/mol	Joback Method
hvap	44.18	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.189		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
tb	424.66	K	Joback Method
tc	596.14	K	Joback Method
tf	186.44	K	Joback Method
vc	0.359	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.29	J/molxK	424.66	Joback Method
cpg	235.79	J/molxK	567.56	Joback Method
cpg	227.84	J/molxK	538.98	Joback Method
cpg	219.53	J/molxK	510.40	Joback Method
cpg	210.84	J/molxK	481.82	Joback Method
cpg	201.77	J/molxK	453.24	Joback Method
cpg	243.39	J/molxK	596.14	Joback Method
dvisc	0.0002336	Paxs	424.66	Joback Method

dvisc	0.0004399	Paxs	384.96	Joback Method
dvisc	0.0009580	Paxs	345.25	Joback Method
dvisc	0.0025541	Paxs	305.55	Joback Method
dvisc	0.0091265	Paxs	265.85	Joback Method
dvisc	0.0510015	Paxs	226.14	Joback Method
dvisc	0.5931093	Paxs	186.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1569591&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

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	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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