3-Methyl-4-penten-2-ol

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

Physical Properties

Property code	Value	Unit	Source
af	0.4761		Cheméo Relay (1.0)
gf	-54.22	kJ/mol	Joback Method
hf	-234.73	kJ/mol	Cheméo Relay (1.0)
hfus	7.06	kJ/mol	Joback Method
hvap	54.54	kJ/mol	Cheméo Relay (1.0)
ie	9.59	eV	Cheméo Relay (1.0)
log10ws	-0.47		Cheméo Relay (1.0)
logp	1.189		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
tb	399.16	K	Cheméo Relay (1.0)
tc	561.33	K	Cheméo Relay (1.0)
tf	217.78	K	Cheméo Relay (1.0)
vc	0.348	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

dvisc	0.5931093	Pa×s	186.44	Joback Method
dvisc	0.0510015	Pa×s	226.14	Joback Method
dvisc	0.0091265	Pa×s	265.85	Joback Method
dvisc	0.0025541	Pa×s	305.55	Joback Method
dvisc	0.0009580	Pa×s	345.25	Joback Method
dvisc	0.0004399	Pa×s	384.96	Joback Method
dvisc	0.0002336	Pa×s	424.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1569591&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 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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