1-Penten-3-ol, 4-methyl-

Other names: 4-methyl-1-penten-3-ol
Inchi: InChI=1S/C6H12O/c1-4-6(7)5(2)3/h4-7H,1H2,2-3H3
InchiKey: SZKVYEHTIWILMA-UHFFFAOYSA-N
Formula: C6H12O
SMILES: C=CC(O)C(C)C
Mol. weight [g/mol]: 100.16
CAS: 4798-45-2

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
rinpol	704.00		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	704.00		NIST Webbook
tb	424.66	K	Joback Method
tc	596.14	K	Joback Method
tf	186.44	K	Joback Method
vc	0.359	m3/kmol	Joback Method

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

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=C4798452&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
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

Latest version available from: