4-Penten-1-ol, 2-methyl-

Other names: 2-methyl-4-penten-1-ol
Inchi: InChI=1S/C6H12O/c1-3-4-6(2)5-7/h3,6-7H,1,4-5H2,2H3
InchiKey: CTHUAOGQNZSMMC-UHFFFAOYSA-N
Formula: C6H12O
SMILES: C=CCC(C)CO
Mol. weight [g/mol]: 100.16
CAS: 5673-98-3

Physical Properties

Property code	Value	Unit	Source
gf	-51.78	kJ/mol	Joback Method
hf	-199.25	kJ/mol	Joback Method
hfus	10.58	kJ/mol	Joback Method
hvap	44.57	kJ/mol	Joback Method
log10ws	-1.21		Crippen Method
logp	1.191		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3664.21	kPa	Joback Method
ripol	1375.00		NIST Webbook
ripol	1375.00		NIST Webbook
tb	425.10	K	Joback Method
tc	592.88	K	Joback Method
tf	201.44	K	Joback Method
vc	0.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.23	J/mol×K	425.10	Joback Method
cpg	234.52	J/mol×K	564.91	Joback Method
cpg	226.77	J/mol×K	536.95	Joback Method
cpg	218.68	J/mol×K	508.99	Joback Method
cpg	210.23	J/mol×K	481.03	Joback Method
cpg	201.41	J/mol×K	453.06	Joback Method

cpg	241.94	J/mol×K	592.88	Joback Method
dvisc	0.0002428	Pa×s	425.10	Joback Method
dvisc	0.0004340	Pa×s	387.82	Joback Method
dvisc	0.0008774	Pa×s	350.55	Joback Method
dvisc	0.0020977	Pa×s	313.27	Joback Method
dvisc	0.0063461	Pa×s	275.99	Joback Method
dvisc	0.0271287	Pa×s	238.72	Joback Method
dvisc	0.1985438	Pa×s	201.44	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50131e+01
Coeff. B	-3.83367e+03
Coeff. C	-5.69790e+01
Temperature range (K), min.	317.32
Temperature range (K), max.	452.13

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5673983&Units=SI

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
pvap:	Vapor pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume