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

Other names: 4-Methyl-3-penten-1-ol
4-Methyl-3-pentenol
4-Methylpent-3-en-1-ol
Inchi: InChI=1S/C6H12O/c1-6(2)4-3-5-7/h4,7H,3,5H2,1-2H3
InchiKey: FKKLUOCEIANSFL-UHFFFAOYSA-N
Formula: C6H12O
SMILES: CC(C)=CCCO
Mol. weight [g/mol]: 100.16
CAS: 763-89-3

Physical Properties

Property code	Value	Unit	Source
gf	-65.51	kJ/mol	Joback Method
hf	-211.97	kJ/mol	Joback Method
hfus	14.28	kJ/mol	Joback Method
hvap	45.67	kJ/mol	Joback Method
log10ws	-1.45		Crippen Method
logp	1.335		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
pc	3695.46	kPa	Joback Method
rinpol	868.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	868.20		NIST Webbook
rinpol	868.20		NIST Webbook
ripol	1390.00		NIST Webbook
ripol	1375.00		NIST Webbook
ripol	1390.00		NIST Webbook
ripol	1390.00		NIST Webbook
ripol	1375.00		NIST Webbook
ripol	1385.00		NIST Webbook
ripol	1375.00		NIST Webbook
tb	430.20	K	NIST Webbook
tc	604.77	K	Joback Method
tf	199.16	K	Joback Method
vc	0.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.73	J/mol×K	432.90	Joback Method
cpg	201.02	J/mol×K	461.54	Joback Method
cpg	209.90	J/mol×K	490.19	Joback Method
cpg	218.38	J/mol×K	518.83	Joback Method
cpg	226.47	J/mol×K	547.48	Joback Method
cpg	234.20	J/mol×K	576.12	Joback Method
cpg	241.57	J/mol×K	604.77	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59066e+01
Coeff. B	-4.17008e+03
Coeff. C	-6.07320e+01
Temperature range (K), min.	295.70
Temperature range (K), max.	454.32

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C763893&Units=SI

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

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume