4-Methyl-4-penten-2-ol

Other names: 4-methylpent-4-en-2-ol
Inchi: InChI=1S/C6H12O/c1-5(2)4-6(3)7/h6-7H,1,4H2,2-3H3
InchiKey: KPHPTSMXBAVNPX-UHFFFAOYSA-N
Formula: C6H12O
SMILES: C=C(C)CC(C)O
Mol. weight [g/mol]: 100.16
CAS: 2004-67-3

Physical Properties

Property code	Value	Unit	Source
hfus	9.27	kJ/mol	Joback Method
hvap	51.31	kJ/mol	Cheméo Relay (1.0)
ie	9.33	eV	Cheméo Relay (1.0)
logp	1.333		Crippen Method
mcvol	96.970	ml/mol	McGowan Method
tb	400.40	K	Cheméo Relay (1.0)
tf	186.29	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.18	J/mol×K	424.98	Joback Method
cpg	201.51	J/mol×K	453.46	Joback Method
cpg	210.45	J/mol×K	481.95	Joback Method
cpg	219.01	J/mol×K	510.43	Joback Method
cpg	227.21	J/mol×K	538.92	Joback Method
cpg	235.05	J/mol×K	567.40	Joback Method
cpg	242.55	J/mol×K	595.89	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40577e+01
Coeff. B	-3.50754e+03
Coeff. C	-5.41990e+01
Temperature range (K), min.	295.70
Temperature range (K), max.	455.23

Sources

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):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2004673&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point