3,4-Dimethyl-1-pentyn-3-ol

Other names: 3,4-Dimethyl-1-penten-3-ol
Inchi: InChI=1S/C7H12O/c1-5-7(4,8)6(2)3/h1,6,8H,2-4H3
InchiKey: DZNLEQBXXLGELU-UHFFFAOYSA-N
Formula: C7H12O
SMILES: C#CC(C)(O)C(C)C
Mol. weight [g/mol]: 112.17
CAS: 1482-15-1

Physical Properties

Property code	Value	Unit	Source
hf	-64.01	kJ/mol	Cheméo Relay (1.0)
hfus	10.01	kJ/mol	Joback Method
hvap	55.77	kJ/mol	Cheméo Relay (1.0)
ie	9.97	eV	Cheméo Relay (1.0)
log10ws	-0.77		Cheméo Relay (1.0)
logp	1.027		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
tb	405.93	K	Cheméo Relay (1.0)
tf	263.35	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.23	J/mol×K	438.19	Joback Method
cpg	231.76	J/mol×K	469.14	Joback Method
cpg	241.68	J/mol×K	500.09	Joback Method
cpg	251.02	J/mol×K	531.04	Joback Method
cpg	259.82	J/mol×K	561.99	Joback Method
cpg	268.10	J/mol×K	592.93	Joback Method
cpg	275.90	J/mol×K	623.88	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64196e+01
Coeff. B	-4.55664e+03
Coeff. C	-6.71610e+01
Temperature range (K), min.	349.15
Temperature range (K), max.	477.15

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):	
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=C1482151&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point