3-Methyl-4-hexyn-3-ol

Inchi: InChI=1S/C7H12O/c1-4-6-7(3,8)5-2/h8H,5H2,1-3H3
InchiKey: VLRDHNINMBNPDK-UHFFFAOYSA-N
Formula: C7H12O
SMILES: CC#CC(C)(O)CC
Mol. weight [g/mol]: 112.17
CAS: 6320-68-9

Physical Properties

Property code	Value	Unit	Source
gf	76.88	kJ/mol	Joback Method
hf	-76.49	kJ/mol	Joback Method
hfus	13.68	kJ/mol	Joback Method
hvap	48.71	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.171		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3815.10	kPa	Joback Method
tb	457.51	K	Joback Method
tc	650.27	K	Joback Method
tf	337.99	K	Joback Method
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.44	J/mol×K	457.51	Joback Method
cpg	230.91	J/mol×K	489.64	Joback Method
cpg	240.81	J/mol×K	521.76	Joback Method
cpg	250.19	J/mol×K	553.89	Joback Method
cpg	259.05	J/mol×K	586.01	Joback Method
cpg	267.43	J/mol×K	618.14	Joback Method
cpg	275.36	J/mol×K	650.27	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

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=C6320689&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume