1-Heptyn-4-ol

Inchi: InChI=1S/C7H12O/c1-3-5-7(8)6-4-2/h1,7-8H,4-6H2,2H3
InchiKey: LYXYBSYXGARUEA-UHFFFAOYSA-N
Formula: C7H12O
SMILES: C#CCC(O)CCC
Mol. weight [g/mol]: 112.17
CAS: 22127-83-9

Physical Properties

Property code	Value	Unit	Source
gf	91.87	kJ/mol	Joback Method
hf	-53.42	kJ/mol	Joback Method
hfus	17.43	kJ/mol	Joback Method
hvap	47.33	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.171		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3708.97	kPa	Joback Method
tb	441.42	K	Joback Method
tc	615.96	K	Joback Method
tf	261.44	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.57	J/mol×K	441.42	Joback Method
cpg	228.02	J/mol×K	470.51	Joback Method
cpg	237.04	J/mol×K	499.60	Joback Method
cpg	245.67	J/mol×K	528.69	Joback Method
cpg	253.91	J/mol×K	557.78	Joback Method
cpg	261.78	J/mol×K	586.87	Joback Method
cpg	269.29	J/mol×K	615.96	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

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=C22127839&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

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