4-Heptyn-2-ol

Other names: hept-4-yn-2-ol
Inchi: InChI=1S/C7H12O/c1-3-4-5-6-7(2)8/h7-8H,3,6H2,1-2H3
InchiKey: CXVIEBMEWKSONY-UHFFFAOYSA-N
Formula: C7H12O
SMILES: CCC#CCC(C)O
Mol. weight [g/mol]: 112.17
CAS: 19781-81-8

Physical Properties

Property code	Value	Unit	Source
gf	71.60	kJ/mol	Joback Method
hf	-73.02	kJ/mol	Joback Method
hfus	17.57	kJ/mol	Joback Method
hvap	49.62	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.171		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3763.78	kPa	Joback Method
tb	460.30	K	Joback Method
tc	645.47	K	Joback Method
tf	320.57	K	Joback Method
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.62	J/mol×K	460.30	Joback Method
cpg	227.38	J/mol×K	491.16	Joback Method
cpg	236.73	J/mol×K	522.02	Joback Method
cpg	245.69	J/mol×K	552.89	Joback Method
cpg	254.28	J/mol×K	583.75	Joback Method
cpg	262.50	J/mol×K	614.61	Joback Method
cpg	270.36	J/mol×K	645.47	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	341.00	K	1.90	NIST Webbook

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=C19781818&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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