2-Heptyn-4-ol

Inchi: InChI=1S/C7H12O/c1-3-5-7(8)6-4-2/h7-8H,3,5H2,1-2H3
InchiKey: AYFRKLSJSAVMRG-UHFFFAOYSA-N
Formula: C7H12O
SMILES: CC#CC(O)CCC
Mol. weight [g/mol]: 112.17

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
rinpol	939.00		NIST Webbook
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

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=R511016&Units=SI
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume