2-Heptyn-1-ol

Other names: hept-2-yn-1-ol
Inchi: InChI=1S/C7H12O/c1-2-3-4-5-6-7-8/h8H,2-4,7H2,1H3
InchiKey: OGDYROFIIXDTQK-UHFFFAOYSA-N
Formula: C7H12O
SMILES: CCCCC#CCO
Mol. weight [g/mol]: 112.17
CAS: 1002-36-4

Physical Properties

Property code	Value	Unit	Source
gf	74.04	kJ/mol	Joback Method
hf	-67.74	kJ/mol	Joback Method
hfus	21.10	kJ/mol	Joback Method
hvap	50.01	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	1.172		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
tb	460.74	K	Joback Method
tc	641.90	K	Joback Method
tf	335.57	K	Joback Method
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.45	J/mol×K	460.74	Joback Method
cpg	226.91	J/mol×K	490.93	Joback Method
cpg	236.00	J/mol×K	521.13	Joback Method
cpg	244.72	J/mol×K	551.32	Joback Method
cpg	253.09	J/mol×K	581.52	Joback Method
cpg	261.11	J/mol×K	611.71	Joback Method
cpg	268.80	J/mol×K	641.90	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C1002364&Units=SI

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