Hex-2-en-4-in-1-ol

Inchi: InChI=1S/C6H8O/c1-2-3-4-5-6-7/h4-5,7H,6H2,1H3/b5-4+
InchiKey: FOQPBGTTZIKXSH-SNAWJCMRSA-N
Formula: C6H8O
SMILES: CC#CC=CCO
Mol. weight [g/mol]: 96.13

Physical Properties

Property code	Value	Unit	Source
gf	145.84	kJ/mol	Joback Method
hf	70.12	kJ/mol	Joback Method
hfus	18.71	kJ/mol	Joback Method
hvap	47.74	kJ/mol	Joback Method
log10ws	-1.25		Crippen Method
logp	0.558		Crippen Method
mcvol	88.370	ml/mol	McGowan Method
pc	4504.30	kPa	Joback Method
ripol	1256.00		NIST Webbook
ripol	1256.00		NIST Webbook
tb	442.02	K	Joback Method
tc	633.84	K	Joback Method
tf	319.22	K	Joback Method
vc	0.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	162.29	J/mol×K	442.02	Joback Method
cpg	170.00	J/mol×K	473.99	Joback Method
cpg	177.33	J/mol×K	505.96	Joback Method
cpg	184.30	J/mol×K	537.93	Joback Method
cpg	190.92	J/mol×K	569.90	Joback Method
cpg	197.21	J/mol×K	601.87	Joback Method
cpg	203.20	J/mol×K	633.84	Joback Method

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=R518755&Units=SI
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume