(Z)-4-hepten-2-ol

Other names: 4-Hepten-2-ol, (Z)-
(Z)-hept-4-en-2-ol
Inchi: InChI=1S/C7H14O/c1-3-4-5-6-7(2)8/h4-5,7-8H,3,6H2,1-2H3/b5-4-
InchiKey: KZUFTCBJDQXWOJ-PLNGDYQASA-N
Formula: C7H14O
SMILES: CCC=CCC(C)O
Mol. weight [g/mol]: 114.19
CAS: 34146-55-9

Physical Properties

Property code	Value	Unit	Source
gf	-50.98	kJ/mol	Joback Method
hf	-228.10	kJ/mol	Joback Method
hfus	14.65	kJ/mol	Joback Method
hvap	47.42	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.723		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
rinpol	869.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	869.00		NIST Webbook
ripol	1310.00		NIST Webbook
ripol	1310.00		NIST Webbook
tb	455.46	K	Joback Method
tc	626.76	K	Joback Method
tf	209.39	K	Joback Method
vc	0.420	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.62	J/mol×K	455.46	Joback Method

cpg	242.14	J/mol×K	484.01	Joback Method
cpg	252.19	J/mol×K	512.56	Joback Method
cpg	261.78	J/mol×K	541.11	Joback Method
cpg	270.95	J/mol×K	569.66	Joback Method
cpg	279.70	J/mol×K	598.21	Joback Method
cpg	288.05	J/mol×K	626.76	Joback Method
dvisc	0.1747804	Pa×s	209.39	Joback Method
dvisc	0.0210963	Pa×s	250.40	Joback Method
dvisc	0.0046173	Pa×s	291.41	Joback Method
dvisc	0.0014702	Pa×s	332.43	Joback Method
dvisc	0.0006019	Pa×s	373.44	Joback Method
dvisc	0.0002941	Pa×s	414.45	Joback Method
dvisc	0.0001634	Pa×s	455.46	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C34146559&Units=SI
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

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume