cis-4-Hepten-2-one

Other names: (Z)-4-hepten-2-one
Inchi: InChI=1S/C7H12O/c1-3-4-5-6-7(2)8/h4-5H,3,6H2,1-2H3/b5-4-
InchiKey: VQKIKHHXFHNXJT-PLNGDYQASA-N
Formula: C7H12O
SMILES: CCC=CCC(C)=O
Mol. weight [g/mol]: 112.17

Physical Properties

Property code	Value	Unit	Source
gf	-40.64	kJ/mol	Joback Method
hf	-183.17	kJ/mol	Joback Method
hfus	15.69	kJ/mol	Joback Method
hvap	37.88	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.932		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3173.97	kPa	Joback Method
rinpol	868.00		NIST Webbook
rinpol	874.00		NIST Webbook
ripol	1230.00		NIST Webbook
tb	417.59	K	Joback Method
tc	603.10	K	Joback Method
tf	213.50	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.10	J/mol×K	417.59	Joback Method
cpg	211.15	J/mol×K	448.51	Joback Method
cpg	221.68	J/mol×K	479.43	Joback Method
cpg	231.70	J/mol×K	510.34	Joback Method
cpg	241.24	J/mol×K	541.26	Joback Method
cpg	250.32	J/mol×K	572.18	Joback Method

cpg	258.95	J/mol×K	603.10	Joback Method
dvisc	0.0038148	Pa×s	213.50	Joback Method
dvisc	0.0017711	Pa×s	247.51	Joback Method
dvisc	0.0009898	Pa×s	281.53	Joback Method
dvisc	0.0006271	Pa×s	315.54	Joback Method
dvisc	0.0004342	Pa×s	349.56	Joback Method
dvisc	0.0003209	Pa×s	383.57	Joback Method
dvisc	0.0002491	Pa×s	417.59	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=R298798&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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