

cis-2-Hepten-4-one

Inchi:	InChI=1S/C7H12O/c1-3-5-7(8)6-4-2/h3,5H,4,6H2,1-2H3/b5-3-
InchiKey:	TXVAOITYBBWKMG-HYXAFXHYSA-N
Formula:	C7H12O
SMILES:	CC=CC(=O)CCC
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	899.00		NIST Webbook
rinpol	902.00		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=R298783&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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