

2-Hepten-4-one

Other names:	hept-2-en-4-one
Inchi:	InChI=1S/C7H12O/c1-3-5-7(8)6-4-2/h3,5H,4,6H2,1-2H3/b5-3+
InchiKey:	TXVAOITYBBWKMG-HWKANZROSA-N
Formula:	C7H12O
SMILES:	CC=CC(=O)CCC
Mol. weight [g/mol]:	112.17
CAS:	4643-25-8

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
ripol	1232.00		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/molxK	417.59	Joback Method
cpg	211.15	J/molxK	448.51	Joback Method
cpg	221.68	J/molxK	479.43	Joback Method
cpg	231.70	J/molxK	510.34	Joback Method
cpg	241.24	J/molxK	541.26	Joback Method
cpg	250.32	J/molxK	572.18	Joback Method
cpg	258.95	J/molxK	603.10	Joback Method

dvisc	0.0038148	Paxs	213.50	Joback Method
dvisc	0.0017711	Paxs	247.51	Joback Method
dvisc	0.0009898	Paxs	281.53	Joback Method
dvisc	0.0006271	Paxs	315.54	Joback Method
dvisc	0.0004342	Paxs	349.56	Joback Method
dvisc	0.0003209	Paxs	383.57	Joback Method
dvisc	0.0002491	Paxs	417.59	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=C4643258&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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

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