

5-methyl-5-hepten-2-one

Inchi:	InChI=1S/C8H14O/c1-4-7(2)5-6-8(3)9/h4H,5-6H2,1-3H3/b7-4+
InchiKey:	UBAUITYZPNZXIM-QPJXVBHSA-N
Formula:	C8H14O
SMILES:	CC=C(C)CCC(C)=O
Mol. weight [g/mol]:	126.20
CAS:	10339-67-0

Physical Properties

Property code	Value	Unit	Source
gf	-40.77	kJ/mol	Joback Method
hf	-213.60	kJ/mol	Joback Method
hfus	16.97	kJ/mol	Joback Method
hvap	40.19	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.322		Crippen Method
mvol	120.850	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
rinpol	1012.00		NIST Webbook
tb	440.35	K	Joback Method
tc	627.87	K	Joback Method
tf	210.81	K	Joback Method
vc	0.470	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.66	J/molxK	440.35	Joback Method
cpg	252.05	J/molxK	471.60	Joback Method
cpg	263.86	J/molxK	502.86	Joback Method
cpg	275.09	J/molxK	534.11	Joback Method
cpg	285.78	J/molxK	565.36	Joback Method
cpg	295.94	J/molxK	596.61	Joback Method
cpg	305.60	J/molxK	627.87	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.32660e+01
Coeff. B	-3.44271e+03
Coeff. C	-6.43930e+01
Temperature range (K), min.	329.66
Temperature range (K), max.	497.19

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R510286&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/54-456-6/5-methyl-5-hepten-2-one.pdf>

Generated by Cheméo on 2024-04-19 01:58:11.015412623 +0000 UTC m=+15781139.935989939.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.