3,3-dimethylcyclohexanone

Inchi: InChI=1S/C8H14O/c1-8(2)5-3-4-7(9)6-8/h3-6H2,1-2H3
InchiKey: ZVJQBBYAVPAFLX-UHFFFAOYSA-N
Formula: C8H14O
SMILES: CC1(C)CCCC(=O)C1
Mol. weight [g/mol]: 126.20
CAS: 2979-19-3

Physical Properties

Property code	Value	Unit	Source
gf	-87.15	kJ/mol	Joback Method
hf	-276.59	kJ/mol	Joback Method
hfus	1.52	kJ/mol	Joback Method
hvap	36.93	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	2.156		Crippen Method
mcvol	114.290	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
rinpol	1036.00		NIST Webbook
tb	470.05	K	Joback Method
tc	700.41	K	Joback Method
tf	279.42	K	Joback Method
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.36	J/mol×K	470.05	Joback Method
cpg	264.46	J/mol×K	508.44	Joback Method
cpg	280.52	J/mol×K	546.84	Joback Method
cpg	295.62	J/mol×K	585.23	Joback Method
cpg	309.86	J/mol×K	623.62	Joback Method
cpg	323.33	J/mol×K	662.01	Joback Method
cpg	336.13	J/mol×K	700.41	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49459e+01
Coeff. B	-3.92833e+03
Coeff. C	-6.71260e+01
Temperature range (K), min.	335.12
Temperature range (K), max.	474.87

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2979193&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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/22-304-9/3-3-dimethylcyclohexanone.pdf

Generated by Cheméo on 2024-10-12 09:43:48.770285739 +0000 UTC m=+3307091.407254989.

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