

Cyclohexanone, 2-butyl-

Other names:	2-butylcyclohexanone 2-n-Butylcyclohexanone
Inchi:	InChI=1S/C10H18O/c1-2-3-6-9-7-4-5-8-10(9)11/h9H,2-8H2,1H3
InchiKey:	POYYYYXPQBFPUKS-UHFFFAOYSA-N
Formula:	C10H18O
SMILES:	CCCCC1CCCCC1=O
Mol. weight [g/mol]:	154.25
CAS:	1126-18-7

Physical Properties

Property code	Value	Unit	Source
gf	-64.82	kJ/mol	Joback Method
hf	-333.11	kJ/mol	Joback Method
hfus	13.00	kJ/mol	Joback Method
hvap	42.53	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	2.936		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
tb	515.57	K	Joback Method
tc	729.05	K	Joback Method
tf	278.06	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.22	J/mol×K	515.57	Joback Method
cpg	357.09	J/mol×K	551.15	Joback Method
cpg	375.07	J/mol×K	586.73	Joback Method
cpg	392.17	J/mol×K	622.31	Joback Method
cpg	408.39	J/mol×K	657.89	Joback Method
cpg	423.72	J/mol×K	693.47	Joback Method
cpg	438.17	J/mol×K	729.05	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.38017e+01
Coeff. B	-3.81923e+03
Coeff. C	-7.49100e+01
Temperature range (K), min.	357.52
Temperature range (K), max.	524.75

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1126187&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/ci990307I
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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

Latest version available from:

<https://www.cheméo.com/cid/67-661-4/Cyclohexanone-2-butyl.pdf>

Generated by Cheméo on 2025-12-17 13:44:15.305065141 +0000 UTC m=+5727252.835105805.

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