2-N-BUTYLCYCLOHEXANONE

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

Physical Properties

Property code	Value	Unit	Source
af	0.4325		Cheméo Relay (1.0)
gf	-64.82	kJ/mol	Joback Method
hf	-309.37	kJ/mol	Cheméo Relay (1.0)
hfus	13.00	kJ/mol	Joback Method
hvap	56.86	kJ/mol	Cheméo Relay (1.0)
ie	9.13	eV	Cheméo Relay (1.0)
log10ws	-2.67		Cheméo Relay (1.0)
logp	2.936		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
tb	494.46	K	Cheméo Relay (1.0)
tc	709.27	K	Cheméo Relay (1.0)
tf	249.69	K	Cheméo Relay (1.0)

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(Pvp) = 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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1126187&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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