3-BUTYL-CYCLOHEXANONE

Other names: 3-Butyl-cyclohexanone
Inchi: InChI=1S/C10H18O/c1-2-3-5-9-6-4-7-10(11)8-9/h9H,2-8H2,1H3
InchiKey: ORIINXCHZXECLA-UHFFFAOYSA-N
Formula: C10H18O
SMILES: CCCCC1CCCC(=O)C1
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
af	0.4531		Cheméo Relay (1.0)
gf	-64.82	kJ/mol	Joback Method
hf	-316.97	kJ/mol	Cheméo Relay (1.0)
hfus	13.00	kJ/mol	Joback Method
hvap	56.53	kJ/mol	Cheméo Relay (1.0)
ie	9.26	eV	Cheméo Relay (1.0)
log10ws	-3.11		Cheméo Relay (1.0)
logp	2.936		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
ripol	1711.00		NIST Webbook
ripol	1711.00		NIST Webbook
tb	501.22	K	Cheméo Relay (1.0)
tc	706.93	K	Cheméo Relay (1.0)
tf	251.32	K	Cheméo Relay (1.0)
vc	0.495	m3/kmol	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

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39178693&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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