1-CYCLOHEXYL-1-BUTANONE

Other names: 1-Cyclohexanol-1-butanone
1-Cyclohexyl-1-butanone
1-cyclohexylbutan-1-one
Inchi: InChI=1S/C10H18O/c1-2-6-10(11)9-7-4-3-5-8-9/h9H,2-8H2,1H3
InchiKey: UYMHLXHLPQIDMA-UHFFFAOYSA-N
Formula: C10H18O
SMILES: CCCC(=O)C1CCCCC1
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
hf	-311.04	kJ/mol	Cheméo Relay (1.0)
hfus	15.09	kJ/mol	Joback Method
hvap	52.31	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.62		Cheméo Relay (1.0)
logp	2.936		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
ripol	1984.00		NIST Webbook
ripol	1984.00		NIST Webbook
tb	486.87	K	Cheméo Relay (1.0)
tf	271.70	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.32	J/mol×K	501.62	Joback Method
cpg	346.66	J/mol×K	536.16	Joback Method
cpg	364.02	J/mol×K	570.70	Joback Method
cpg	380.44	J/mol×K	605.24	Joback Method
cpg	395.94	J/mol×K	639.78	Joback Method
cpg	410.54	J/mol×K	674.32	Joback Method
cpg	424.28	J/mol×K	708.86	Joback Method
dvisc	0.0059552	Pa×s	259.77	Joback Method
dvisc	0.0025735	Pa×s	300.08	Joback Method

dvisc	0.0013566	Pa×s	340.39	Joback Method
dvisc	0.0008190	Pa×s	380.69	Joback Method
dvisc	0.0005446	Pa×s	421.00	Joback Method
dvisc	0.0003889	Pa×s	461.31	Joback Method
dvisc	0.0002931	Pa×s	501.62	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	367.20	K	1.70	NIST Webbook

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):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1462277&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point