4-Butyl-cyclohexen-3-one

Inchi: InChI=1S/C10H16O/c1-2-3-4-9-5-7-10(11)8-6-9/h5H,2-4,6-8H2,1H3
InchiKey: IDKGUPRQRXCLKC-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CCCCC1=CCC(=O)CC1
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	-36.78	kJ/mol	Joback Method
hf	-266.46	kJ/mol	Joback Method
hfus	12.76	kJ/mol	Joback Method
hvap	43.79	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.856		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
ripol	1717.00		NIST Webbook
ripol	1717.00		NIST Webbook
tb	524.38	K	Joback Method
tc	741.30	K	Joback Method
tf	295.58	K	Joback Method
vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	320.22	J/mol×K	524.38	Joback Method
cpg	337.15	J/mol×K	560.53	Joback Method
cpg	353.25	J/mol×K	596.69	Joback Method
cpg	368.54	J/mol×K	632.84	Joback Method
cpg	383.01	J/mol×K	668.99	Joback Method
cpg	396.68	J/mol×K	705.15	Joback Method
cpg	409.55	J/mol×K	741.30	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R408707&Units=SI

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