3-Butoxy-2,2-dimethylcyclobutanone

Inchi: InChI=1S/C10H18O2/c1-4-5-6-12-9-7-8(11)10(9,2)3/h9H,4-7H2,1-3H3
InchiKey: KMPAHCHXLPFRLX-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: CCCCOC1CC(=O)C1(C)C
Mol. weight [g/mol]: 170.25
CAS: 2292-83-3

Physical Properties

Property code	Value	Unit	Source
gf	-158.82	kJ/mol	Joback Method
hf	-458.11	kJ/mol	Joback Method
hfus	13.16	kJ/mol	Joback Method
hvap	43.14	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	2.171		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
tb	525.02	K	Joback Method
tc	729.68	K	Joback Method
tf	326.99	K	Joback Method
vc	0.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.52	J/mol×K	525.02	Joback Method
cpg	381.24	J/mol×K	559.13	Joback Method
cpg	397.16	J/mol×K	593.24	Joback Method
cpg	412.33	J/mol×K	627.35	Joback Method
cpg	426.83	J/mol×K	661.46	Joback Method
cpg	440.72	J/mol×K	695.57	Joback Method
cpg	454.06	J/mol×K	729.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2292833&Units=SI
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

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