

Cyclohexanone-1,3-butanediol ketal

Inchi: InChI=1S/C9H16O2/c1-8-7-10-9(11-8)5-3-2-4-6-9/h8H,2-7H2,1H3
InchiKey: LKGNKCNAPNUZCM-UHFFFAOYSA-N
Formula: C9H16O2
SMILES: CC1COC2(CCCCC2)O1
Mol. weight [g/mol]: 156.22

Physical Properties

Property code	Value	Unit	Source
gf	-79.73	kJ/mol	Joback Method
hf	-356.89	kJ/mol	Joback Method
hfus	16.60	kJ/mol	Joback Method
hvap	44.01	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	2.082		Crippen Method
mcvol	127.690	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
rinpol	1186.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1500.00		NIST Webbook
tb	490.02	K	Joback Method
tc	722.61	K	Joback Method
tf	290.03	K	Joback Method
vc	0.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.75	J/mol×K	490.02	Joback Method
cpg	327.69	J/mol×K	528.79	Joback Method
cpg	346.12	J/mol×K	567.55	Joback Method
cpg	363.20	J/mol×K	606.32	Joback Method
cpg	379.09	J/mol×K	645.08	Joback Method
cpg	393.94	J/mol×K	683.85	Joback Method
cpg	407.92	J/mol×K	722.61	Joback Method

Sources

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=R409606&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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