Cyclohexanone, 4-(1,1-dimethylethyl)-2-ethyl-, cis-

Inchi: InChI=1S/C12H22O/c1-5-9-8-10(12(2,3)4)6-7-11(9)13/h9-10H,5-8H2,1-4H3/t9-,10-/m0/s1

InchiKey: UMEJTHPXAININP-UWVGGRQHSA-N

Formula: C12H22O

SMILES: CCC1CC(C(C)(C)C)CCC1=O

Mol. weight [g/mol]: 182.30

CAS: 32188-05-9

Physical Properties

Property code	Value	Unit	Source
gf	-52.85	kJ/mol	Joback Method
hf	-403.48	kJ/mol	Joback Method
hfus	11.84	kJ/mol	Joback Method
hvap	45.38	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.428		Crippen Method
mcvol	170.650	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
tb	553.43	K	Joback Method
tc	773.08	K	Joback Method
tf	298.78	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.52	J/mol×K	553.43	Joback Method
cpg	462.55	J/mol×K	590.04	Joback Method
cpg	483.35	J/mol×K	626.65	Joback Method
cpg	502.95	J/mol×K	663.26	Joback Method
cpg	521.38	J/mol×K	699.87	Joback Method
cpg	538.65	J/mol×K	736.48	Joback Method
cpg	554.78	J/mol×K	773.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32188059&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

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