2-hexylcyclohexan-1-one

Other names: 2-Cyclohexylcyclohexanone
Inchi: InChI=1S/C12H20O/c13-12-9-5-4-8-11(12)10-6-2-1-3-7-10/h10-11H,1-9H2
InchiKey: UOBQDYFTAJKQAL-UHFFFAOYSA-N
Formula: C12H22O
SMILES: O=C1CCCCC1C1CCCCC1
Mol. weight [g/mol]: 182.30
CAS: 24848-00-8

Physical Properties

Property code	Value	Unit	Source
gf	-23.53	kJ/mol	Joback Method
hf	-320.07	kJ/mol	Joback Method
hfus	10.02	kJ/mol	Joback Method
hvap	47.41	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.326		Crippen Method
mcvol	159.790	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
tb	580.88	K	Joback Method
tc	828.16	K	Joback Method
tf	307.98	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.54	J/mol×K	580.88	Joback Method
cpg	453.38	J/mol×K	622.09	Joback Method
cpg	476.60	J/mol×K	663.31	Joback Method
cpg	498.22	J/mol×K	704.52	Joback Method
cpg	518.25	J/mol×K	745.73	Joback Method
cpg	536.71	J/mol×K	786.95	Joback Method
cpg	553.62	J/mol×K	828.16	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	430.00 ± 1.00	K	2.90	NIST Webbook

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=C24848008&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume