2-Benzylcyclohexanone

Other names: Cyclohexanone, 2-(phenylmethyl)-
2-benzylcyclohexan-1-one
Inchi: InChI=1S/C13H16O/c14-13-9-5-4-8-12(13)10-11-6-2-1-3-7-11/h1-3,6-7,12H,4-5,8-10H2
InchiKey: CUYLPYBYCYQGCE-UHFFFAOYSA-N
Formula: C13H16O
SMILES: O=C1CCCCC1Cc1ccccc1
Mol. weight [g/mol]: 188.27
CAS: 946-33-8

Physical Properties

Property code	Value	Unit	Source
gf	72.85	kJ/mol	Joback Method
hf	-158.50	kJ/mol	Joback Method
hfus	14.81	kJ/mol	Joback Method
hvap	51.48	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.988		Crippen Method
mcvol	160.980	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
tb	610.89	K	Joback Method
tc	861.11	K	Joback Method
tf	338.29	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.44	J/mol×K	610.89	Joback Method
cpg	438.10	J/mol×K	652.59	Joback Method
cpg	457.29	J/mol×K	694.30	Joback Method
cpg	475.03	J/mol×K	736.00	Joback Method
cpg	491.36	J/mol×K	777.71	Joback Method
cpg	506.30	J/mol×K	819.41	Joback Method
cpg	519.88	J/mol×K	861.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C946338&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