3-Phenylcyclobutanone

Inchi: InChI=1S/C10H10O/c11-10-6-9(7-10)8-4-2-1-3-5-8/h1-5,9H,6-7H2
InchiKey: BVQSFCUGCAZOJQ-UHFFFAOYSA-N
Formula: C10H10O
SMILES: O=C1CC(c2ccccc2)C1
Mol. weight [g/mol]: 146.19
CAS: 52784-31-3

Physical Properties

Property code	Value	Unit	Source
chl	-5307.80 ± 1.50	kJ/mol	NIST Webbook
gf	71.79	kJ/mol	Joback Method
hf	-84.26	kJ/mol	Joback Method
hfl	-56.57	kJ/mol	NIST Webbook
hfus	11.24	kJ/mol	Joback Method
hvap	46.40 ± 0.80	kJ/mol	NIST Webbook
log10ws	-2.25		Crippen Method
logp	2.133		Crippen Method
mcvol	118.710	ml/mol	McGowan Method
pc	3642.13	kPa	Joback Method
tb	533.71	K	Joback Method
tc	782.10	K	Joback Method
tf	311.52	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.06	J/mol×K	533.71	Joback Method
cpg	286.50	J/mol×K	575.11	Joback Method
cpg	301.82	J/mol×K	616.51	Joback Method
cpg	316.06	J/mol×K	657.90	Joback Method
cpg	329.25	J/mol×K	699.30	Joback Method
cpg	341.45	J/mol×K	740.70	Joback Method
cpg	352.67	J/mol×K	782.10	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52784313&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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