

3-Phenyl-1-indanone

Other names:	3-Phenylindan-1-one 1-Indanone, 3-phenyl- 1H-Inden-1-one, 2,3-dihydro-3-phenyl- 1H-Indene-1-one, 2,3-dihydro-3-phenyl-
Inchi:	InChI=1S/C15H12O/c16-15-10-14(11-6-2-1-3-7-11)12-8-4-5-9-13(12)15/h1-9,14H,10H2
InchiKey:	SIUOTMYWHGODQX-UHFFFAOYSA-N
Formula:	C15H12O
SMILES:	O=C1CC(c2ccccc2)c2ccccc21
Mol. weight [g/mol]:	208.26
CAS:	16618-72-7

Physical Properties

Property code	Value	Unit	Source
gf	228.77	kJ/mol	Joback Method
hf	43.76	kJ/mol	Joback Method
hfus	19.94	kJ/mol	Joback Method
hvap	58.36	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.405		Crippen Method
mcvol	165.400	ml/mol	McGowan Method
pc	2934.52	kPa	Joback Method
tb	675.50	K	Joback Method
tc	941.52	K	Joback Method
tf	410.33	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.43	J/molxK	675.50	Joback Method
cpg	452.76	J/molxK	719.84	Joback Method
cpg	468.61	J/molxK	764.17	Joback Method
cpg	483.08	J/molxK	808.51	Joback Method
cpg	496.27	J/molxK	852.85	Joback Method

cpg	508.25	J/mol×K	897.19	Joback Method
cpg	519.14	J/mol×K	941.52	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	474.50 ± 1.50	K	2.10	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16618727&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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