

Cyclohexene, 1-phenyl-

Other names:	Benzene, 1-cyclohexen-1-yl- 1-Phenyl-1-cyclohexene 1-Phenylcyclohexene Phenyl-1-cyclohexene cyclohexen-1-ylbenzene
Inchi:	InChI=1S/C12H14/c1-3-7-11(8-4-1)12-9-5-2-6-10-12/h1,3-4,7-9H,2,5-6,10H2
InchiKey:	WCMSFBRREKZZFL-UHFFFAOYSA-N
Formula:	C12H14
SMILES:	C1=C(c2ccccc2)CCCC1
Mol. weight [g/mol]:	158.24
CAS:	771-98-2

Physical Properties

Property code	Value	Unit	Source
chl	-6706.10 ± 6.70	kJ/mol	NIST Webbook
gf	215.06	kJ/mol	Joback Method
hf	66.49	kJ/mol	Joback Method
hfus	12.47	kJ/mol	Joback Method
hvap	46.27	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.644		Crippen Method
mcvol	141.020	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
rinpol	1384.00		NIST Webbook
rinpol	1384.00		NIST Webbook
rinpol	1384.00		NIST Webbook
tb	525.20	K	NIST Webbook
tc	773.62	K	Joback Method
tf	276.32	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	314.64	J/mol×K	529.00	Joback Method
cpg	396.85	J/mol×K	732.85	Joback Method
cpg	382.91	J/mol×K	692.08	Joback Method
cpg	367.79	J/mol×K	651.31	Joback Method
cpg	351.42	J/mol×K	610.54	Joback Method
cpg	333.73	J/mol×K	569.77	Joback Method
cpg	409.68	J/mol×K	773.62	Joback Method
dvisc	0.0002021	Pa×s	529.00	Joback Method
dvisc	0.0002668	Pa×s	486.89	Joback Method
dvisc	0.0003713	Pa×s	444.77	Joback Method
dvisc	0.0005536	Pa×s	402.66	Joback Method
dvisc	0.0009061	Pa×s	360.55	Joback Method
dvisc	0.0016896	Pa×s	318.43	Joback Method
dvisc	0.0038097	Pa×s	276.32	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	398.70	K	1.90	NIST Webbook

Sources

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=C771982&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
rinpol:	Non-polar retention indices
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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