

Cyclohexanol, 1-phenyl-

Other names:	Cyclohexanol, 1-phenyl- 1-Phenyl-1-cyclohexanol 1-Phenylcyclohexanol-1 Benzene, cyclohex-1-yl-1-ol-
Inchi:	InChI=1S/C12H16O/c13-12(9-5-2-6-10-12)11-7-3-1-4-8-11/h1,3-4,7-8,13H,2,5-6,9-10H2
InchiKey:	DTTDXHDYTWQDCS-UHFFFAOYSA-N
Formula:	C12H16O
SMILES:	OC1(c2ccccc2)CCCCC1
Mol. weight [g/mol]:	176.26

Physical Properties

Property code	Value	Unit	Source
hf	-153.14	kJ/mol	Cheméo Relay (1.0)
hfus	10.50	kJ/mol	Joback Method
ie	8.00	eV	NIST Webbook
logp	2.838		Crippen Method
mcvol	151.190	ml/mol	McGowan Method
tb	537.49	K	Cheméo Relay (1.0)
tf	333.00 ± 4.00	K	NIST Webbook
tf	333.00 ± 3.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.22	J/mol×K	612.61	Joback Method
cpg	410.80	J/mol×K	650.86	Joback Method
cpg	426.27	J/mol×K	689.11	Joback Method
cpg	440.80	J/mol×K	727.36	Joback Method
cpg	454.54	J/mol×K	765.61	Joback Method
cpg	467.65	J/mol×K	803.87	Joback Method
cpg	480.29	J/mol×K	842.12	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1589602&Units=SI
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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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