

1H-Imidazole, 4,5-dihydro-2-(phenylmethyl)-

Other names:	2-Imidazoline, 2-benzyl- Artonil Benzazoline Benzidazol Benzolin Benzylimidazoline Dilatol ASI Divascol Imidalin Kasimid Lambril Olitensol Peripherine Phenylmethylimidazoline Prefaxil Priscol Priscoline Tolazolin Tolazoline Vasimid Vasodil Vasodilatan 2-Benzyl-2-imidazoline 2-Benzyl-4,5-imidazoline 2-Benzylimidazoline CIBA 3259 Imidaline 4,5-Dihydro-2-(phenylmethyl)-1H-imidazole Benzolin (vasodilator) NSC 35110
Inchi:	InChI=1S/C10H12N2/c1-2-4-9(5-3-1)8-10-11-6-7-12-10/h1-5H,6-8H2,(H,11,12)
InchiKey:	JIVZKJJQOZQXQB-UHFFFAOYSA-N
Formula:	C10H12N2
SMILES:	<chem>c1ccc(CC2=NCCN2)cc1</chem>
Mol. weight [g/mol]:	160.22
CAS:	59-98-3

Physical Properties

Property code	Value	Unit	Source
gf	414.81	kJ/mol	Joback Method
hf	222.71	kJ/mol	Joback Method
hfus	24.12	kJ/mol	Joback Method
hvap	54.62	kJ/mol	Joback Method
ie	8.50	eV	NIST Webbook
log10ws	-1.85		Crippen Method
logp	1.231		Crippen Method
mcvol	132.800	ml/mol	McGowan Method
pc	3970.51	kPa	Joback Method
rinpol	1471.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1477.00		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1510.00		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	1477.00		NIST Webbook
tb	581.22	K	Joback Method
tc	839.25	K	Joback Method
tf	433.87	K	Joback Method
vc	0.501	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.16	J/mol×K	581.22	Joback Method
cpg	343.65	J/mol×K	624.22	Joback Method
cpg	359.83	J/mol×K	667.23	Joback Method
cpg	374.72	J/mol×K	710.23	Joback Method
cpg	388.37	J/mol×K	753.24	Joback Method
cpg	400.83	J/mol×K	796.24	Joback Method

Sources

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=C59983&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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