Bendazole

Other names:	1H-Benzimidazole, 2-(phenylmethyl)-
	2-(Phenylmethyl)-1H-benzimidazole
	2-Benzylbenzimidazole
	2-Benzylbenziminazole
	Benzimidazole, 2-benzyl-
	Dibasol
	Dibazol
	Dibazole
	NSC 60020
	Tromasedan
	bendazol
Inchi:	InChI=1S/C14H12N2/c1-2-6-11(7-3-1)10-14-15-12-8-4-5-9-13(12)16-14/h1-9H,10H2,(H,1
InchiKey:	YTLQFZVCLXFFRK-UHFFFAOYSA-N
Formula:	C14H12N2
SMILES:	c1ccc(Cc2nc3ccccc3[nH]2)cc1
Mol. weight [g/mol]:	208.26

Physical Properties

Property code	Value	Unit	Source
af	0.5294		Cheméo Relay (1.0)
hf	289.94	kJ/mol	Cheméo Relay (1.0)
hsub	136.20 ± 0.50	kJ/mol	NIST Webbook
hvap	97.30	kJ/mol	Cheméo Relay (1.0)
ie	8.15	eV	Cheméo Relay (1.0)
log10ws	-3.55		Cheméo Relay (1.0)
logp	2.672		Crippen Method
mcvol	165.400	ml/mol	McGowan Method
pc	4068.34	kPa	Cheméo Relay (1.0, beta)
tb	643.49	K	Cheméo Relay (1.0)
tc	942.56	K	Cheméo Relay (1.0)
tf	570.50	K	Thermochemical properties of two benzimidazole derivatives: 2-Phenyl- and 2-benzylbenzimidazole
vc	0.635	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	134.50 ± 0.50	kJ/mol	402.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Thermochemical properties of two benzimidazole derivatives: 2-Phenyl- and 2-benzylbenzimidazole:	https://www.doi.org/10.1016/j.jct.2005.02.008
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C621727&Units=SI

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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