Naphazoline

Other names:	1H-Imidazole, 4,5-dihydro-2-(1-naphthalenylmethyl)-
	2-Imidazoline, 2-(1-naphthylmethyl)-
	Antan
	Imidin
	Naphthizine
	Rhinazine
	2-(1-Naphthylmethyl)-2-imidazoline
	CIBA 2020/r
	2-(Naphthyl-(1')-methyl)imidazolin
	«alpha»-Naphthylmethyl imidazoline
	2-(«alpha»-Naphthylmethyl)-imidazoline
	2-(1-Naphthalenylmethyl)-2-imidazoline
Inchi:	InChI=1S/C14H14N2/c1-2-7-13-11(4-1)5-3-6-12(13)10-14-15-8-9-16-14/h1-7H,8-10H2,(H
InchiKey:	CNIIGCLFLJGOGP-UHFFFAOYSA-N
Formula:	C14H14N2
SMILES:	c1ccc2c(CC3=NCCN3)cccc2c1
Mol. weight [g/mol]:	210.27
CAS:	835-31-4

Physical Properties

Property code	Value	Unit	Source
gf	545.51	kJ/mol	Joback Method
hf	319.75	kJ/mol	Joback Method
hfus	31.11	kJ/mol	Joback Method
hvap	65.82	kJ/mol	Joback Method
ie	8.46	eV	NIST Webbook
log10ws	-3.66		Crippen Method
logp	2.384		Crippen Method
mcvol	169.700	ml/mol	McGowan Method
pc	3299.15	kPa	Joback Method
rinpol	1990.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1993.00		NIST Webbook
rinpol	1993.00		NIST Webbook
tb	696.70	K	Joback Method
tc	964.62	K	Joback Method
tf	524.17	K	Joback Method

vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.76	J/mol×K	696.70	Joback Method
cpg	483.21	J/mol×K	741.35	Joback Method
cpg	499.12	J/mol×K	786.01	Joback Method
cpg	513.62	J/mol×K	830.66	Joback Method
cpg	526.79	J/mol×K	875.32	Joback Method
cpg	538.73	J/mol×K	919.97	Joback Method
cpg	549.56	J/mol×K	964.62	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=C835314&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume