

Aprindine

Other names:

1,3-Propanediamine, N-(2,3-dihydro-1H-inden-2-yl)-N',N'-diethyl-N-phenyl-
N,N-Diethyl-N'-2-indanyl-N'-phenyl-1,3-propanediamine
AC-1802
Compd 99170
Lilly 99170

Inchi:

N-(2,3-Dihydro-1H-inden-2-yl)-N',N'-diethyl-N-phenyl-1,3-propanediamine

InchiKey:

NZLBHDRPUJLHCE-UHFFFAOYSA-N

Formula:

C22H30N2

SMILES:

CCN(CC)CCCN(c1ccccc1)C1Cc2ccccc2C1

Mol. weight [g/mol]:

322.49

CAS:

37640-71-4

Physical Properties

Property code	Value	Unit	Source
gf	631.86	kJ/mol	Joback Method
hf	172.04	kJ/mol	Joback Method
hfus	44.61	kJ/mol	Joback Method
hvap	73.78	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.392		Crippen Method
mcvol	282.420	ml/mol	McGowan Method
pc	1529.46	kPa	Joback Method
rinpol	2480.00		NIST Webbook
rinpol	2460.00		NIST Webbook
tb	792.72	K	Joback Method
tc	1009.27	K	Joback Method
tf	485.94	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.85	J/molxK	792.72	Joback Method

cpg	891.62	J/mol×K	828.81	Joback Method
cpg	910.10	J/mol×K	864.90	Joback Method
cpg	927.42	J/mol×K	900.99	Joback Method
cpg	943.71	J/mol×K	937.08	Joback Method
cpg	959.11	J/mol×K	973.18	Joback Method
cpg	973.72	J/mol×K	1009.27	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C37640714&Units=SI

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
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

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