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 N-(2,3-Dihydro-1H-inden-2-yl)-N',N'-diethyl-N-phenyl-1,3-propanediamine
Inchi:	InChI=1S/C22H30N2/c1-3-23(4-2)15-10-16-24(21-13-6-5-7-14-21)22-17-19-11-8-9-12-20
InchiKey:	NZLBHDRPUJLHCE-UHFFFAOYSA-N
Formula:	C22H30N2
SMILES:	CCN(CC)CCCN(c1ccccc1)C1Cc2ccccc2C1
Mol. weight [g/mol]:	322.50

Physical Properties

Property code	Value	Unit	Source
hfus	44.61	kJ/mol	Joback Method
logp	4.392		Crippen Method
mcvol	282.420	ml/mol	McGowan Method
rinpol	2480.00		NIST Webbook
rinpol	2480.00		NIST Webbook
rinpol	2460.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.85	J/mol×K	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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C37640714&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices