Alverine

Other names:	Benzenepropanamine, N-ethyl-N-(3-phenylpropyl)-
	Bis(«gamma»-phenylpropyl)ethylamine
	Dipropylamine, N-ethyl-3,3'-diphenyl-
	Dipropylin
	Dipropyline
	N-Ethyl-3,3'-diphenyldipropylamine
	N-ethyl-3-phenyl-N-(3-phenylpropyl)propan-1-amine
	N-ethyl-N-(3-phenylpropyl)-benzenepropanamine
	Phenopropamine
	Phenpropamine
	Profenil
	Sestron
	Sestron base
Inchi:	InChI=1S/C20H27N/c1-2-21(17-9-15-19-11-5-3-6-12-19)18-10-16-20-13-7-4-8-14-20/h3-
InchiKey:	ZPFXAOWNKLFJDN-UHFFFAOYSA-N
Formula:	C20H27N
SMILES:	CCN(CCCc1ccccc1)CCCc1ccccc1
Mol. weight [g/mol]:	281.44
CAS:	150-59-4

Physical Properties

Property code	Value	Unit	Source
gf	453.12	kJ/mol	Joback Method
hf	84.46	kJ/mol	Joback Method
hfus	38.66	kJ/mol	Joback Method
hvap	66.71	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.574		Crippen Method
mcvol	255.120	ml/mol	McGowan Method
pc	1628.54	kPa	Joback Method
rinpol	2142.00		NIST Webbook
rinpol	2137.00		NIST Webbook
rinpol	2145.00		NIST Webbook
rinpol	2142.00		NIST Webbook
tb	722.80	K	Joback Method
tc	934.70	K	Joback Method
tf	400.47	K	Joback Method

vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.92	J/mol×K	899.39	Joback Method
cpg	729.40	J/mol×K	722.80	Joback Method
cpg	748.95	J/mol×K	758.12	Joback Method
cpg	767.18	J/mol×K	793.43	Joback Method
cpg	784.20	J/mol×K	828.75	Joback Method
cpg	800.09	J/mol×K	864.07	Joback Method
cpg	828.78	J/mol×K	934.70	Joback Method
hvapt	89.30	kJ/mol	298.00	Evaluation of the Vaporization Enthalpies and Liquid Vapor Pressures of (R)-Deprenyl, (S)-Benzphetamine, Alverine, and a Series of Aliphatic Tertiary Amines by Correlation Gas Chromatography at T/K = 298.15

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C150594&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Evaluation of the Vaporization Enthalpies and Liquid Vapor Pressures of (R)-Deprenyl, (S)-Benzphetamine, Alverine, and a Series of Aliphatic Tertiary Amines by Correlation Gas Chromatography at T/K = 298.15:	https://www.doi.org/10.1021/je500358r
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvapt:	Enthalpy of vaporization at a given temperature
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