Phentermine

Other names:	.alpha.,.alpha.-dimethylbenzeneethanamine
	1,1-dimethyl-2-phenylethylamine
	2-Phenyl-tert-butylamine
	2-methyl-1-phenylpropan-2-amine
	Apidex P
	Benzeneethanamine, alpha,alpha-dimethyl-
	Benzeneethanamine, «alpha»,«alpha»-dimethyl-
	Benzethanamine, «alpha»,«alpha»-dimethyl
	Duromine
	Ethanamine, 1,1-dimethyl-2-phenyl-
	Inoamin
	Ionamin
	Linyl
	Lipopill
	Lonamin
	Mirapront
	Normephentermine
	Omnibex
	Phenethylamine, «alpha»,«alpha»-dimethyl-
	Phenyl-tert-butylamine
	Rcra waste number P046
	Wilpo
	«alpha»,«alpha»-Dimethyl-«beta»-phenylethylamine
	«alpha»,«alpha»-Dimethylbenzeneethanamine
	«alpha»,«alpha»-Dimethylphenethylamine
	«alpha»-Benzylisopropylamine
Inchi:	InChI=1S/C10H15N/c1-10(2,11)8-9-6-4-3-5-7-9/h3-7H,8,11H2,1-2H3
InchiKey:	DHHVAGZRUROJKS-UHFFFAOYSA-N
Formula:	C10H15N
SMILES:	CC(C)(N)Cc1ccccc1
Mol. weight [g/mol]:	149.23
CAS:	122-09-8

Physical Properties

Property code	Value	Unit	Source
gf	215.02	kJ/mol	Joback Method

hf	11.84	kJ/mol	Joback Method
hfus	13.48	kJ/mol	Joback Method
hvap	49.47	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	1.966		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
pc	3188.33	kPa	Joback Method
rinpol	195.47		NIST Webbook
rinpol	195.74		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1173.40		NIST Webbook
rinpol	1159.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1177.00		NIST Webbook
rinpol	1183.00		NIST Webbook
rinpol	1191.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1138.00		NIST Webbook
ripol	1566.00		NIST Webbook
ripol	1573.00		NIST Webbook
ripol	1573.00		NIST Webbook
ripol	1629.00		NIST Webbook
ripol	1649.00		NIST Webbook
ripol	1638.00		NIST Webbook
tb	524.18	K	Joback Method
tc	754.29	K	Joback Method
tf	314.56	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.43	J/mol×K	524.18	Joback Method
cpg	335.58	J/mol×K	562.53	Joback Method
cpg	350.55	J/mol×K	600.88	Joback Method
cpg	364.41	J/mol×K	639.23	Joback Method
cpg	377.24	J/mol×K	677.58	Joback Method
cpg	389.10	J/mol×K	715.93	Joback Method
cpg	400.07	J/mol×K	754.29	Joback Method
pvap	0.04	kPa	298.15	The Vaporization Enthalpies and Vapor Pressures of Some Primary Amines of Pharmaceutical Importance by Correlation Gas Chromatography

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C122098&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The Vaporization Enthalpies and Vapor Pressures of Some Primary Amines of Pharmaceutical Importance by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je400498a
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
log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume