

Benzeneethanamine, .alpha.,.alpha.-dimethyl-

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 phentermine «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:	DHHVAGZRURJKS-UHFFFAOYSA-N
Formula:	C10H15N
SMILES:	CC(C)(N)Cc1ccccc1
Mol. weight [g/mol]:	149.24

Physical Properties

Property code	Value	Unit	Source
af	0.4675		Cheméo Relay (1.0)

gf	215.02	kJ/mol	Joback Method
hf	10.02	kJ/mol	Cheméo Relay (1.0)
hfus	13.48	kJ/mol	Joback Method
hvap	57.77	kJ/mol	Cheméo Relay (1.0)
ie	8.47	eV	Cheméo Relay (1.0)
log10ws	-2.01		Cheméo Relay (1.0)
logp	1.966		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
pc	3188.33	kPa	Joback Method
rinpol	1183.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1130.00		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	1174.00		NIST Webbook
rinpol	1191.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	195.74		NIST Webbook
rinpol	195.47		NIST Webbook
rinpol	1155.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1155.00		NIST Webbook
ripol	1649.00		NIST Webbook
ripol	1638.00		NIST Webbook
ripol	1629.00		NIST Webbook
ripol	1566.00		NIST Webbook
ripol	1573.00		NIST Webbook
ripol	1573.00		NIST Webbook
tb	478.33	K	Cheméo Relay (1.0)
tc	695.40	K	Cheméo Relay (1.0)

tf	266.31	K	Cheméo Relay (1.0)
vc	0.499	m3/kmol	Cheméo Relay (1.0)

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>

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):

The Vaporization Enthalpies and Vapor Pressures of Some Primary Amines of Pharmaceutical Importance by Correlation Gas Chromatography: <https://www.doi.org/10.1021/je400498a>

Legend

af: Acentric Factor

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
pvap:	Vapor pressure
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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