Benzphetamine

Other names:	Benzeneethanamine, N,«alpha»-dimethyl-N-(phenylmethyl)-, (+)-
	Phenethylamine, N-benzyl-N,«alpha»-dimethyl-, (+)-
	N-Benzyl-N,«alpha»-dimethylphenethylamine
	Benzaphetamine
	Benzfetamine
	d-Benzphetamine
	N-Benzylmethamphetamine
	(+)-Benzphetamine
	5411-22-3 (hydrochloride)
Inchi:	InChI=1S/C17H21N/c1-15(13-16-9-5-3-6-10-16)18(2)14-17-11-7-4-8-12-17/h3-12,15H,13
InchiKey:	YXKTVDFXDRQTKV-UHFFFAOYSA-N
Formula:	C17H21N
SMILES:	CC(Cc1ccccc1)N(C)Cc1ccccc1
Mol. weight [g/mol]:	239.36
CAS:	156-08-1

Physical Properties

Property code	Value	Unit	Source
gf	425.42	kJ/mol	Joback Method
hf	141.10	kJ/mol	Joback Method
hfus	27.37	kJ/mol	Joback Method
hvap	59.64	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.750		Crippen Method
mcvol	212.850	ml/mol	McGowan Method
pc	2100.34	kPa	Joback Method
rinpol	1807.00		NIST Webbook
rinpol	1850.00		NIST Webbook
rinpol	1855.00		NIST Webbook
rinpol	1806.00		NIST Webbook
rinpol	1855.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1834.00		NIST Webbook
rinpol	1855.00		NIST Webbook
rinpol	1850.00		NIST Webbook
ripol	2392.00		NIST Webbook
ripol	2392.00		NIST Webbook

tb	653.72	K	Joback Method
tc	880.44	K	Joback Method
tf	351.66	K	Joback Method
vc	0.783	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.96	J/mol×K	653.72	Joback Method
cpg	583.53	J/mol×K	691.51	Joback Method
cpg	601.67	J/mol×K	729.29	Joback Method
cpg	618.47	J/mol×K	767.08	Joback Method
cpg	634.02	J/mol×K	804.86	Joback Method
cpg	648.41	J/mol×K	842.65	Joback Method
cpg	661.74	J/mol×K	880.44	Joback Method

Sources

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=C156081&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume