Benzphentermine

Inchi: InChI=1S/C17H21N/c1-17(2,13-15-9-5-3-6-10-15)18-14-16-11-7-4-8-12-16/h3-12,18H,13
InchiKey: WUWANIZIMGVMSA-UHFFFAOYSA-N
Formula: C17H21N
SMILES: CC(C)(Cc1ccccc1)NCc1ccccc1
Mol. weight [g/mol]: 239.36

Physical Properties

Property code	Value	Unit	Source
gf	409.31	kJ/mol	Joback Method
hf	123.57	kJ/mol	Joback Method
hfus	25.55	kJ/mol	Joback Method
hvap	63.13	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	3.797		Crippen Method
mcvol	212.850	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
rinpol	1858.00		NIST Webbook
rinpol	1760.00		NIST Webbook
rinpol	1858.00		NIST Webbook
rinpol	1760.00		NIST Webbook
tb	688.66	K	Joback Method
tc	925.53	K	Joback Method
tf	389.27	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.77	J/mol×K	688.66	Joback Method
cpg	602.50	J/mol×K	728.14	Joback Method
cpg	619.76	J/mol×K	767.62	Joback Method
cpg	635.65	J/mol×K	807.10	Joback Method
cpg	650.30	J/mol×K	846.58	Joback Method
cpg	663.83	J/mol×K	886.05	Joback Method

cpg	676.35	J/mol×K	925.53	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=R17216&Units=SI

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