N-Benzylamphetamine

Other names: Benzylamphetamine
Inchi: InChI=1S/C16H19N/c1-14(12-15-8-4-2-5-9-15)17-13-16-10-6-3-7-11-16/h2-11,14,17H,12
InchiKey: JLCDKDGHTWGGQM-UHFFFAOYSA-N
Formula: C16H19N
SMILES: CC(Cc1ccccc1)NCc1ccccc1
Mol. weight [g/mol]: 225.33
CAS: 57378-23-1

Physical Properties

Property code	Value	Unit	Source
gf	395.61	kJ/mol	Joback Method
hf	147.68	kJ/mol	Joback Method
hfus	26.85	kJ/mol	Joback Method
hvap	61.81	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.407		Crippen Method
mcvol	198.760	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
rinpol	1784.00		NIST Webbook
rinpol	1784.00		NIST Webbook
rinpol	1784.00		NIST Webbook
ripol	2390.00		NIST Webbook
ripol	2390.00		NIST Webbook
ripol	2390.00		NIST Webbook
tb	668.57	K	Joback Method
tc	901.43	K	Joback Method
tf	360.58	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.13	J/mol×K	668.57	Joback Method
cpg	546.26	J/mol×K	707.38	Joback Method

cpg	563.04	J/mol×K	746.19	Joback Method
cpg	578.54	J/mol×K	785.00	Joback Method
cpg	592.85	J/mol×K	823.81	Joback Method
cpg	606.06	J/mol×K	862.62	Joback Method
cpg	618.24	J/mol×K	901.43	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57378231&Units=SI

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

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