Benzeneethanamine, N-ethyl-N,«alpha»-dimethyl-

Other names: Ethyl-methylamphetamine
Methylethylamphetamine
N-Ethyl-N-methylamphetamine
N-Methyl,N-ethyl-amphetamine

Inchi: InChI=1S/C12H19N/c1-4-13(3)11(2)10-12-8-6-5-7-9-12/h5-9,11H,4,10H2,1-3H3

InchiKey: RGXSEQYXMRRSTM-UHFFFAOYSA-N

Formula: C12H19N

SMILES: CCN(C)C(C)Cc1ccccc1

Mol. weight [g/mol]: 177.29

CAS: 119290-77-6

Physical Properties

Property code	Value	Unit	Source
gf	270.91	kJ/mol	Joback Method
hf	7.77	kJ/mol	Joback Method
hfus	20.38	kJ/mol	Joback Method
hvap	46.24	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.569		Crippen Method
mcvol	166.160	ml/mol	McGowan Method
pc	2419.50	kPa	Joback Method
rinpol	1320.00		NIST Webbook
rinpol	1320.00		NIST Webbook
ripol	1609.00		NIST Webbook
ripol	1609.00		NIST Webbook
tb	512.64	K	Joback Method
tc	713.65	K	Joback Method
tf	268.89	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.39	J/mol×K	512.64	Joback Method

cpg	398.35	J/mol×K	546.14	Joback Method
cpg	415.29	J/mol×K	579.64	Joback Method
cpg	431.25	J/mol×K	613.14	Joback Method
cpg	446.26	J/mol×K	646.65	Joback Method
cpg	460.38	J/mol×K	680.15	Joback Method
cpg	473.64	J/mol×K	713.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C119290776&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

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