

Benzeneethanamine, «alpha»-methyl-N-(1-methylethyl)-

Other names:	Isopropylamphetamine N-Isopropyl-1-phenyl-2-propanamine N-Isopropylamphetamine
Inchi:	InChI=1S/C12H19N/c1-10(2)13-11(3)9-12-7-5-4-6-8-12/h4-8,10-11,13H,9H2,1-3H3
InchiKey:	PJXXJRMRFYMEY-UHFFFAOYSA-N
Formula:	C12H19N
SMILES:	CC(C)NC(C)Cc1ccccc1
Mol. weight [g/mol]:	177.29
CAS:	33236-69-0

Physical Properties

Property code	Value	Unit	Source
gf	247.08	kJ/mol	Joback Method
hf	-11.57	kJ/mol	Joback Method
hfus	18.93	kJ/mol	Joback Method
hvap	50.24	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	2.616		Crippen Method
mcvol	166.160	ml/mol	McGowan Method
pc	2475.19	kPa	Joback Method
rinpol	1257.00		NIST Webbook
rinpol	1253.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1247.00		NIST Webbook
rinpol	1253.00		NIST Webbook
ripol	1552.00		NIST Webbook
ripol	1552.00		NIST Webbook
tb	549.93	K	Joback Method
tc	758.97	K	Joback Method
tf	274.08	K	Joback Method
vc	0.623	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.96	J/mol×K	549.93	Joback Method
cpg	416.46	J/mol×K	584.77	Joback Method
cpg	432.94	J/mol×K	619.61	Joback Method
cpg	448.43	J/mol×K	654.45	Joback Method
cpg	462.98	J/mol×K	689.29	Joback Method
cpg	476.63	J/mol×K	724.13	Joback Method
cpg	489.42	J/mol×K	758.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33236690&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

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