Benzeneacetonitrile, .alpha.-[(1-methyl-2-phenylethyl)amino]-

Other names: Benzeneacetonitrile, «alpha»-[(1-methyl-2-phenylethyl)amino]-
Amfetaminil
Acetonitrile, [(«alpha»-methylphenethyl)amino]phenyl-
«alpha»-Phenyl-«alpha»-(1-phenylisopropyl)aminoacetonitrile
dl-Amphetaminil
Aponeuron
AN 1
AN 1 (pharmaceutical)
N-(«beta»-Phenylisopropyl)-«alpha»-aminophenylacetonitrile
N-(«alpha»-Methylphenethyl)-2-phenylglycinonitrile
«alpha»-Phenyl-«alpha»-(1-methyl-2-phenyl)ethylaminoacetonitrile
«alpha»-Phenyl-«alpha»(«beta»-phenylisopropylamino)acetonitrile
«alpha»-Phenyl-«alpha»-N-(1-phenylisopropyl)aminoacetonitrile
[(«alpha»-Methylphenethyl)amino]phenylacetonitrile
NSC 67172

Inchi: InChI=1S/C17H18N2/c1-14(12-15-8-4-2-5-9-15)19-17(13-18)16-10-6-3-7-11-16/h2-11,14

InchiKey: NFHVTCJKAHYEQN-UHFFFAOYSA-N

Formula: C17H18N2

SMILES: CC(Cc1ccccc1)NC(C#N)c1ccccc1

Mol. weight [g/mol]: 250.35

Physical Properties

Property code	Value	Unit	Source
af	0.5561		Cheméo Relay (1.0)
hf	263.94	kJ/mol	Cheméo Relay (1.0)
hfus	27.43	kJ/mol	Joback Method
hvap	96.99	kJ/mol	Cheméo Relay (1.0)
ie	8.68	eV	Cheméo Relay (1.0)
log10ws	-2.99		Cheméo Relay (1.0)
logp	3.472		Crippen Method
mcvol	214.230	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
tb	611.21	K	Cheméo Relay (1.0)
tc	899.32	K	Cheméo Relay (1.0)
tf	345.94	K	Cheméo Relay (1.0)
vc	0.750	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.15	J/mol×K	793.09	Joback Method
cpg	624.93	J/mol×K	833.63	Joback Method
cpg	638.48	J/mol×K	874.17	Joback Method
cpg	650.90	J/mol×K	914.72	Joback Method
cpg	662.29	J/mol×K	955.26	Joback Method
cpg	672.74	J/mol×K	995.80	Joback Method
cpg	682.35	J/mol×K	1036.34	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17590011&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature

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