Amphetaminil

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]: 250.34

CAS: 17590-01-1

Physical Properties

Property code	Value	Unit	Source
gf	534.77	kJ/mol	Joback Method
hf	286.64	kJ/mol	Joback Method
hfus	27.43	kJ/mol	Joback Method
hvap	74.13	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	3.472		Crippen Method
mcvol	214.230	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
tb	793.09	K	Joback Method
tc	1036.34	K	Joback Method
tf	421.84	K	Joback Method
vc	0.821	m3/kmol	Joback Method

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

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=C17590011&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume