Benzeneacetonitrile, «alpha»-phenyl-

Other names:	Acetonitrile, diphenyl-
	«alpha»-Phenylbenzylcyanide
	«alpha»-Phenylphenylacetonitrile
	Benzhydrylcyanide
	Dipan
	Diphenatrile
	Diphenyl-«alpha»-cyanomethane
	Diphenylacetonitrile
	Diphenylmethylcyanide
	USAF KF-13
	Benzyhydrylcyanide
	«alpha»-Cyanodiphenylmethane
	Difenylacetonitril
	alpha-Phenylbenzyl cyanide
	alpha-Phenylphenylacetonitrile
	Diphenyl-alpha-cyanomethane
	«alpha»-Phenyl-benzeneacetonitrile
	NSC 130268
Inchi:	InChI=1S/C14H11N/c15-11-14(12-7-3-1-4-8-12)13-9-5-2-6-10-13/h1-10,14H
InchiKey:	NEBPTMCRLHKPOB-UHFFFAOYSA-N
Formula:	C14H11N
SMILES:	N#CC(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	193.24
CAS:	86-29-3

Physical Properties

Property code	Value	Unit	Source
gf	422.56	kJ/mol	Joback Method
hf	300.37	kJ/mol	Joback Method
hfus	18.08	kJ/mol	Joback Method
hvap	61.40	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.342		Crippen Method
mcvol	161.980	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
tb	674.72	K	Joback Method
tc	932.92	K	Joback Method

tf	350.37	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.81	J/mol×K	674.72	Joback Method
cpg	415.07	J/mol×K	717.75	Joback Method
cpg	428.07	J/mol×K	760.79	Joback Method
cpg	439.89	J/mol×K	803.82	Joback Method
cpg	450.64	J/mol×K	846.86	Joback Method
cpg	460.40	J/mol×K	889.89	Joback Method
cpg	469.28	J/mol×K	932.92	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	454.20	K	1.60	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C86293&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume