

Glycinonitrile, 2,2-diphenyl-

Inchi:	InChI=1S/C14H12N2/c15-11-14(16,12-7-3-1-4-8-12)13-9-5-2-6-10-13/h1-10H,16H2
InchiKey:	XLHAFLQPSYZDOK-UHFFFAOYSA-N
Formula:	C14H12N2
SMILES:	N#CC(N)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	208.26
CAS:	52460-99-8

Physical Properties

Property code	Value	Unit	Source
gf	494.29	kJ/mol	Joback Method
hf	330.69	kJ/mol	Joback Method
hfus	19.39	kJ/mol	Joback Method
hvap	71.13	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	2.412		Crippen Method
mcvol	171.960	ml/mol	McGowan Method
pc	2925.00	kPa	Joback Method
tb	744.46	K	Joback Method
tc	1017.09	K	Joback Method
tf	451.05	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.24	J/molxK	744.46	Joback Method
cpg	472.32	J/molxK	789.90	Joback Method
cpg	484.11	J/molxK	835.34	Joback Method
cpg	494.76	J/molxK	880.78	Joback Method
cpg	504.43	J/molxK	926.21	Joback Method
cpg	513.29	J/molxK	971.65	Joback Method
cpg	521.49	J/molxK	1017.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52460998&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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