

Vinylphenylacetonitrile

Inchi:	InChI=1S/C10H9N/c1-2-9-4-3-5-10(8-9)6-7-11/h2-5,8H,1,6H2
InchiKey:	VBRWJLQEFUANAQ-UHFFFAOYSA-N
Formula:	C10H9N
SMILES:	<chem>C=Cc1cccc(CC#N)c1</chem>
Mol. weight [g/mol]:	143.19
CAS:	110013-89-3

Physical Properties

Property code	Value	Unit	Source
gf	357.12	kJ/mol	Joback Method
hf	265.64	kJ/mol	Joback Method
hfus	15.53	kJ/mol	Joback Method
hvap	50.60	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.396		Crippen Method
mcvol	125.080	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
tb	558.62	K	Joback Method
tc	787.94	K	Joback Method
tf	304.63	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.32	J/molxK	558.62	Joback Method
cpg	279.77	J/molxK	596.84	Joback Method
cpg	290.45	J/molxK	635.06	Joback Method
cpg	300.41	J/molxK	673.28	Joback Method
cpg	309.68	J/molxK	711.50	Joback Method
cpg	318.31	J/molxK	749.72	Joback Method
cpg	326.33	J/molxK	787.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110013893&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
mccvol:	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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