

Dibenzylamine, n-isobutenyl-

Inchi:	InChI=1S/C18H21N/c1-16(2)13-19(14-17-9-5-3-6-10-17)15-18-11-7-4-8-12-18/h3-13H,14
InchiKey:	SRGBGKAKYZDTFD-UHFFFAOYSA-N
Formula:	C18H21N
SMILES:	CC(C)=CN(Cc1ccccc1)Cc1ccccc1
Mol. weight [g/mol]:	251.37
CAS:	88893-11-2

Physical Properties

Property code	Value	Unit	Source
gf	507.95	kJ/mol	Joback Method
hf	233.17	kJ/mol	Joback Method
hfus	32.37	kJ/mol	Joback Method
hvap	62.30	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	4.612		Crippen Method
mcvol	222.640	ml/mol	McGowan Method
pc	2012.70	kPa	Joback Method
tb	681.08	K	Joback Method
tc	911.88	K	Joback Method
tf	358.89	K	Joback Method
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.19	J/molxK	681.08	Joback Method
cpg	614.31	J/molxK	719.55	Joback Method
cpg	632.02	J/molxK	758.01	Joback Method
cpg	648.41	J/molxK	796.48	Joback Method
cpg	663.61	J/molxK	834.94	Joback Method
cpg	677.74	J/molxK	873.41	Joback Method
cpg	690.91	J/molxK	911.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88893112&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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