

«alpha»-Benzylphenethylamine

Other names:	2-Propanamine, 1,3-diphenyl
Inchi:	InChI=1S/C15H17N/c16-15(11-13-7-3-1-4-8-13)12-14-9-5-2-6-10-14/h1-10,15H,11-12,16
InchiKey:	BWYYVSNVUCFQQN-UHFFFAOYSA-N
Formula:	C15H17N
SMILES:	NC(Cc1ccccc1)Cc1ccccc1
Mol. weight [g/mol]:	211.30

Physical Properties

Property code	Value	Unit	Source
gf	364.25	kJ/mol	Joback Method
hf	148.64	kJ/mol	Joback Method
hfus	24.36	kJ/mol	Joback Method
hvap	63.79	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	2.799		Crippen Method
mcvol	184.670	ml/mol	McGowan Method
pc	2681.86	kPa	Joback Method
rinpol	1800.00		NIST Webbook
rinpol	1800.00		NIST Webbook
tb	668.05	K	Joback Method
tc	914.23	K	Joback Method
tf	379.91	K	Joback Method
vc	0.682	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.66	J/mol×K	668.05	Joback Method
cpg	504.02	J/mol×K	709.08	Joback Method
cpg	519.99	J/mol×K	750.11	Joback Method
cpg	534.66	J/mol×K	791.14	Joback Method
cpg	548.13	J/mol×K	832.17	Joback Method
cpg	560.48	J/mol×K	873.20	Joback Method
cpg	571.82	J/mol×K	914.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U335157&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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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