2-benzylpiperidine

Inchi: InChI=1S/C12H17N/c1-2-6-11(7-3-1)10-12-8-4-5-9-13-12/h1-3,6-7,12-13H,4-5,8-10H2
InchiKey: ITXCORRITGNIHP-UHFFFAOYSA-N
Formula: C12H17N
SMILES: c1ccc(CC2CCCCN2)cc1
Mol. weight [g/mol]: 175.27
CAS: 32838-55-4

Physical Properties

Property code	Value	Unit	Source
gf	274.73	kJ/mol	Joback Method
hf	37.65	kJ/mol	Joback Method
hfus	22.30	kJ/mol	Joback Method
hvap	51.77	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.371		Crippen Method
mcvol	155.300	ml/mol	McGowan Method
pc	3055.79	kPa	Joback Method
tb	568.74	K	Joback Method
tc	813.54	K	Joback Method
tf	305.00	K	NIST Webbook
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.33	J/mol×K	568.74	Joback Method
cpg	402.18	J/mol×K	609.54	Joback Method
cpg	421.58	J/mol×K	650.34	Joback Method
cpg	439.58	J/mol×K	691.14	Joback Method
cpg	456.24	J/mol×K	731.94	Joback Method
cpg	471.61	J/mol×K	772.74	Joback Method
cpg	485.75	J/mol×K	813.54	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	462.00	K	1.60	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32838554&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