Phenylpropylmethylamine

Other names: Phenpromethamine
Inchi: InChI=1S/C10H15N/c1-10(2,8-11)9-6-4-3-5-7-9/h3-7H,8,11H2,1-2H3
InchiKey: CWSGTPMVOJFVIF-UHFFFAOYSA-N
Formula: C10H15N
SMILES: CC(C)(CN)c1ccccc1
Mol. weight [g/mol]: 149.23
CAS: 93-88-9

Physical Properties

Property code	Value	Unit	Source
gf	215.02	kJ/mol	Joback Method
hf	11.84	kJ/mol	Joback Method
hfus	13.48	kJ/mol	Joback Method
hvap	49.47	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	1.923		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
pc	3188.33	kPa	Joback Method
rinpol	1176.00		NIST Webbook
tb	480.70	K	NIST Webbook
tc	754.29	K	Joback Method
tf	314.56	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.43	J/mol×K	524.18	Joback Method
cpg	335.58	J/mol×K	562.53	Joback Method
cpg	350.55	J/mol×K	600.88	Joback Method
cpg	364.41	J/mol×K	639.23	Joback Method
cpg	377.24	J/mol×K	677.58	Joback Method
cpg	389.10	J/mol×K	715.93	Joback Method
cpg	400.07	J/mol×K	754.29	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	368.70	K	2.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93889&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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