

N-benzylmethylamino-acetone

Inchi:	InChI=1S/C11H15NO/c1-10(13)8-12(2)9-11-6-4-3-5-7-11/h3-7H,8-9H2,1-2H3
InchiKey:	BKBKJBOVLPZZIU-UHFFFAOYSA-N
Formula:	C11H15NO
SMILES:	CC(=O)CN(C)Cc1ccccc1
Mol. weight [g/mol]:	177.24
CAS:	23982-57-2

Physical Properties

Property code	Value	Unit	Source
gf	136.01	kJ/mol	Joback Method
hf	-78.89	kJ/mol	Joback Method
hfus	22.91	kJ/mol	Joback Method
hvap	51.14	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	1.707		Crippen Method
mcvol	153.640	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
tb	544.07	K	Joback Method
tc	752.53	K	Joback Method
tf	322.55	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.38	J/molxK	544.07	Joback Method
cpg	371.81	J/molxK	578.81	Joback Method
cpg	386.29	J/molxK	613.56	Joback Method
cpg	399.85	J/molxK	648.30	Joback Method
cpg	412.53	J/molxK	683.04	Joback Method
cpg	424.39	J/molxK	717.79	Joback Method
cpg	435.45	J/molxK	752.53	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23982572&Units=SI

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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