2-(1-Methylcyclopropyl)aniline

Inchi: InChI=1S/C10H13N/c1-10(6-7-10)8-4-2-3-5-9(8)11/h2-5H,6-7,11H2,1H3
InchiKey: OEFXKZHXLSCUEQ-UHFFFAOYSA-N
Formula: C10H13N
SMILES: CC1(c2ccccc2N)CC1
Mol. weight [g/mol]: 147.22
CAS: 71759-33-6

Physical Properties

Property code	Value	Unit	Source
gf	257.81	kJ/mol	Joback Method
hf	97.16	kJ/mol	Joback Method
hfus	12.34	kJ/mol	Joback Method
hvap	50.20	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.320		Crippen Method
mcvol	127.120	ml/mol	McGowan Method
pc	3763.78	kPa	Joback Method
rinpol	1330.90		NIST Webbook
rinpol	1330.90		NIST Webbook
tb	539.37	K	Joback Method
tc	783.64	K	Joback Method
tf	366.50	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.02	J/mol×K	539.37	Joback Method
cpg	316.18	J/mol×K	580.08	Joback Method
cpg	330.08	J/mol×K	620.79	Joback Method
cpg	342.93	J/mol×K	661.51	Joback Method
cpg	354.92	J/mol×K	702.22	Joback Method
cpg	366.28	J/mol×K	742.93	Joback Method
cpg	377.22	J/mol×K	783.64	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71759336&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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