Sec-butylaminoacetonitrile

Inchi: InChI=1S/C6H12N2/c1-3-6(2)8-5-4-7/h6,8H,3,5H2,1-2H3
InchiKey: OEHOCCGKJKWJAZ-UHFFFAOYSA-N
Formula: C6H12N2
SMILES: CCC(C)NCC#N
Mol. weight [g/mol]: 112.17
CAS: 56095-81-9

Physical Properties

Property code	Value	Unit	Source
gf	219.77	kJ/mol	Joback Method
hf	45.90	kJ/mol	Joback Method
hfus	14.38	kJ/mol	Joback Method
hvap	45.48	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	0.898		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
tb	488.49	K	Joback Method
tc	684.38	K	Joback Method
tf	260.03	K	Joback Method
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.39	J/mol×K	488.49	Joback Method
cpg	240.61	J/mol×K	521.14	Joback Method
cpg	250.36	J/mol×K	553.79	Joback Method
cpg	259.64	J/mol×K	586.44	Joback Method
cpg	268.47	J/mol×K	619.09	Joback Method
cpg	276.87	J/mol×K	651.74	Joback Method
cpg	284.84	J/mol×K	684.38	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=C56095819&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume