isopropyl-n-amylamine

Inchi: InChI=1S/C8H19N/c1-4-5-6-7-9-8(2)3/h8-9H,4-7H2,1-3H3
InchiKey: QCWXZFZXEGTLOV-UHFFFAOYSA-N
Formula: C8H19N
SMILES: CCCCCNC(C)C
Mol. weight [g/mol]: 129.24
CAS: 36343-02-9

Physical Properties

Property code	Value	Unit	Source
gf	103.43	kJ/mol	Joback Method
hf	-160.26	kJ/mol	Joback Method
hfus	18.05	kJ/mol	Joback Method
hvap	39.45	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	2.175		Crippen Method
mcvol	133.560	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	893.00		NIST Webbook
rinpol	893.00		NIST Webbook
tb	432.17	K	Joback Method
tc	604.23	K	Joback Method
tf	217.58	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.40	J/mol×K	432.17	Joback Method
cpg	293.41	J/mol×K	460.85	Joback Method
cpg	306.87	J/mol×K	489.52	Joback Method
cpg	319.80	J/mol×K	518.20	Joback Method
cpg	332.20	J/mol×K	546.88	Joback Method
cpg	344.10	J/mol×K	575.56	Joback Method
cpg	355.50	J/mol×K	604.23	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=C36343029&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