1-Pentanamine, 1-methyl, N-propyl

Inchi: InChI=1S/C9H21N/c1-4-6-7-9-10(3)8-5-2/h4-9H2,1-3H3
InchiKey: OOVHIYXQHWBXPE-UHFFFAOYSA-N
Formula: C9H21N
SMILES: CCCCCN(C)CCC
Mol. weight [g/mol]: 143.27

Physical Properties

Property code	Value	Unit	Source
gf	135.68	kJ/mol	Joback Method
hf	-161.56	kJ/mol	Joback Method
hfus	22.09	kJ/mol	Joback Method
hvap	37.67	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.518		Crippen Method
mcvol	147.650	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
rinpol	977.00		NIST Webbook
rinpol	977.00		NIST Webbook
tb	417.76	K	Joback Method
tc	579.60	K	Joback Method
tf	223.66	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.35	J/mol×K	417.76	Joback Method
cpg	318.41	J/mol×K	444.73	Joback Method
cpg	332.88	J/mol×K	471.71	Joback Method
cpg	346.79	J/mol×K	498.68	Joback Method
cpg	360.15	J/mol×K	525.66	Joback Method
cpg	372.97	J/mol×K	552.63	Joback Method
cpg	385.27	J/mol×K	579.60	Joback Method

Sources

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=R19626&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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