3-Propyl-piperidine

Inchi: InChI=1S/C8H17N/c1-2-4-8-5-3-6-9-7-8/h8-9H,2-7H2,1H3
InchiKey: CRZUKKNUMNKBFJ-UHFFFAOYSA-N
Formula: C8H17N
SMILES: CCCC1CCCNC1
Mol. weight [g/mol]: 127.23
CAS: 13603-14-0

Physical Properties

Property code	Value	Unit	Source
gf	128.64	kJ/mol	Joback Method
hf	-116.32	kJ/mol	Joback Method
hfus	17.90	kJ/mol	Joback Method
hvap	40.59	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	1.786		Crippen Method
mcvol	122.700	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
rinpol	1012.00		NIST Webbook
tb	450.54	K	Joback Method
tc	659.37	K	Joback Method
tf	292.33	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.94	J/mol×K	450.54	Joback Method
cpg	275.63	J/mol×K	485.34	Joback Method
cpg	292.49	J/mol×K	520.15	Joback Method
cpg	308.53	J/mol×K	554.95	Joback Method
cpg	323.77	J/mol×K	589.76	Joback Method
cpg	338.23	J/mol×K	624.56	Joback Method
cpg	351.91	J/mol×K	659.37	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=C13603140&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