2,4,6-Trimethylpiperidine

Inchi: InChI=1S/C8H17N/c1-6-4-7(2)9-8(3)5-6/h6-9H,4-5H2,1-3H3
InchiKey: GELXVDNNZSIRQA-UHFFFAOYSA-N
Formula: C8H17N
SMILES: CC1CC(C)NC(C)C1
Mol. weight [g/mol]: 127.23
CAS: 21974-48-1

Physical Properties

Property code	Value	Unit	Source
gf	113.22	kJ/mol	Joback Method
hf	-157.00	kJ/mol	Joback Method
hfus	20.04	kJ/mol	Joback Method
hvap	39.97	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	1.783		Crippen Method
mcvol	122.700	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
tb	441.20	K	Joback Method
tc	649.34	K	Joback Method
tf	283.85	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.28	J/mol×K	441.20	Joback Method
cpg	276.60	J/mol×K	475.89	Joback Method
cpg	294.15	J/mol×K	510.58	Joback Method
cpg	310.95	J/mol×K	545.27	Joback Method
cpg	326.99	J/mol×K	579.96	Joback Method
cpg	342.28	J/mol×K	614.65	Joback Method
cpg	356.81	J/mol×K	649.34	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.34660e+01
Coeff. B	-3.28964e+03
Coeff. C	-5.73960e+01
Temperature range (K), min.	272.15
Temperature range (K), max.	460.81

Sources

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=C21974481&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume