3-Ethyl-pyrrolidine

Other names: Pyrrolidine, 3-ethyl
Inchi: InChI=1S/C6H13N/c1-2-6-3-4-7-5-6/h6-7H,2-5H2,1H3
InchiKey: DZFFQSFNUBWNSF-UHFFFAOYSA-N
Formula: C6H13N
SMILES: CCC1CCNC1
Mol. weight [g/mol]: 99.17

Physical Properties

Property code	Value	Unit	Source
gf	123.90	kJ/mol	Joback Method
hf	-68.88	kJ/mol	Joback Method
hfus	14.82	kJ/mol	Joback Method
hvap	35.97	kJ/mol	Joback Method
log10ws	-1.18		Crippen Method
logp	1.006		Crippen Method
mcvol	94.520	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
rinpol	841.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	841.00		NIST Webbook
tb	400.51	K	Joback Method
tc	605.61	K	Joback Method
tf	273.31	K	Joback Method
vc	0.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.11	J/mol×K	400.51	Joback Method
cpg	190.42	J/mol×K	434.69	Joback Method
cpg	204.06	J/mol×K	468.88	Joback Method
cpg	217.07	J/mol×K	503.06	Joback Method
cpg	229.45	J/mol×K	537.24	Joback Method
cpg	241.21	J/mol×K	571.43	Joback Method

cpg	252.38	J/mol×K	605.61	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=R405882&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