Heptanenitrile, 3-ethyl-

Inchi: InChI=1S/C9H17N/c1-3-5-6-9(4-2)7-8-10/h9H,3-7H2,1-2H3
InchiKey: SNZMXYKDANOXRV-UHFFFAOYSA-N
Formula: C9H17N
SMILES: CCCCC(CC)CC#N
Mol. weight [g/mol]: 139.24
CAS: 2571-05-3

Physical Properties

Property code	Value	Unit	Source
gf	155.64	kJ/mol	Joback Method
hf	-69.49	kJ/mol	Joback Method
hfus	17.05	kJ/mol	Joback Method
hvap	45.72	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	3.116		Crippen Method
mcvol	139.050	ml/mol	McGowan Method
pc	2269.73	kPa	Joback Method
tb	506.96	K	Joback Method
tc	694.00	K	Joback Method
tf	241.18	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.40	J/mol×K	506.96	Joback Method
cpg	327.33	J/mol×K	538.13	Joback Method
cpg	339.69	J/mol×K	569.31	Joback Method
cpg	351.49	J/mol×K	600.48	Joback Method
cpg	362.76	J/mol×K	631.65	Joback Method
cpg	373.50	J/mol×K	662.83	Joback Method
cpg	383.73	J/mol×K	694.00	Joback Method

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=C2571053&Units=SI
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume