3-Methylpentanenitrile

Inchi: InChI=1S/C6H11N/c1-3-6(2)4-5-7/h6H,3-4H2,1-2H3
InchiKey: MMRQLDRBAXLMRH-UHFFFAOYSA-N
Formula: C6H11N
SMILES: CCC(C)CC#N
Mol. weight [g/mol]: 97.16
CAS: 21101-88-2

Physical Properties

Property code	Value	Unit	Source
gf	130.38	kJ/mol	Joback Method
hf	-7.57	kJ/mol	Joback Method
hfus	9.28	kJ/mol	Joback Method
hvap	39.04	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.946		Crippen Method
mcvol	96.780	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
ripol	1241.00		NIST Webbook
ripol	1241.00		NIST Webbook
tb	438.32	K	Joback Method
tc	631.63	K	Joback Method
tf	207.37	K	Joback Method
vc	0.392	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.99	J/mol×K	438.32	Joback Method
cpg	199.58	J/mol×K	470.54	Joback Method
cpg	208.77	J/mol×K	502.76	Joback Method
cpg	217.55	J/mol×K	534.97	Joback Method
cpg	225.93	J/mol×K	567.19	Joback Method
cpg	233.94	J/mol×K	599.41	Joback Method
cpg	241.57	J/mol×K	631.63	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45973e+01
Coeff. B	-3.64611e+03
Coeff. C	-5.96200e+01
Temperature range (K), min.	314.42
Temperature range (K), max.	452.27

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=R576271&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume