Propanenitrile-25

Inchi: InChI=1S/C3H5N/c1-2-3-4/h2H2,1H3/i1D3,2D2
InchiKey: FVSKHRXBFJPNKK-ZBJDZAJPSA-N
Formula: C3D5N
SMILES: CCC#N
Mol. weight [g/mol]: 60.11
CAS: 10419-75-7

Physical Properties

Property code	Value	Unit	Source
gf	107.56	kJ/mol	Joback Method
hf	59.63	kJ/mol	Joback Method
hfus	5.03	kJ/mol	Joback Method
hvap	32.75	kJ/mol	Joback Method
ie	11.75 ± 0.05	eV	NIST Webbook
log10ws	-0.94		Crippen Method
logp	0.920		Crippen Method
mcvol	54.510	ml/mol	McGowan Method
pc	4266.28	kPa	Joback Method
tb	370.12	K	Joback Method
tc	563.45	K	Joback Method
tf	188.56	K	Joback Method
vc	0.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	86.00	J/mol×K	370.12	Joback Method
cpg	90.77	J/mol×K	402.34	Joback Method
cpg	95.36	J/mol×K	434.56	Joback Method
cpg	99.78	J/mol×K	466.78	Joback Method
cpg	104.02	J/mol×K	499.00	Joback Method
cpg	108.09	J/mol×K	531.23	Joback Method
cpg	112.00	J/mol×K	563.45	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=C10419757&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
ie:	Ionization energy
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