3-Methoxypropionitrile

Inchi: InChI=1S/C4H7NO/c1-6-4-2-3-5/h2,4H2,1H3
InchiKey: OOWFYDWAMOKVSF-UHFFFAOYSA-N
Formula: C4H7NO
SMILES: COCCC#N
Mol. weight [g/mol]: 85.10
CAS: 33695-59-9

Physical Properties

Property code	Value	Unit	Source
chl	-2457.50 ± 0.40	kJ/mol	NIST Webbook
gf	10.98	kJ/mol	Joback Method
hf	-93.23	kJ/mol	Joback Method
hfl	-116.90 ± 0.40	kJ/mol	NIST Webbook
hfus	8.81	kJ/mol	Joback Method
hvap	37.39	kJ/mol	Joback Method
log10ws	-0.45		Crippen Method
logp	0.546		Crippen Method
mcvol	74.470	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
tb	415.42	K	Joback Method
tc	607.19	K	Joback Method
tf	222.06	K	Joback Method
vc	0.303	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.15	J/mol×K	415.42	Joback Method
cpg	143.44	J/mol×K	447.38	Joback Method
cpg	149.56	J/mol×K	479.34	Joback Method
cpg	155.51	J/mol×K	511.31	Joback Method
cpg	161.26	J/mol×K	543.27	Joback Method
cpg	166.84	J/mol×K	575.23	Joback Method
cpg	172.21	J/mol×K	607.19	Joback Method

hvapt	47.60	kJ/mol	383.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54768e+01
Coeff. B	-4.30703e+03
Coeff. C	-4.10490e+01
Temperature range (K), min.	324.61
Temperature range (K), max.	464.75

Sources

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=C33695599&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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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