Propanenitrile, 2-methyl-3-methoxy

Inchi: InChI=1S/C5H9NO/c1-5(3-6)4-7-2/h5H,4H2,1-2H3
InchiKey: ZGQCHFHNSDAMCY-UHFFFAOYSA-N
Formula: C5H9NO
SMILES: COCC(C)C#N
Mol. weight [g/mol]: 99.13

Physical Properties

Property code	Value	Unit	Source
gf	16.96	kJ/mol	Joback Method
hf	-119.15	kJ/mol	Joback Method
hfus	7.88	kJ/mol	Joback Method
hvap	39.22	kJ/mol	Joback Method
log10ws	-0.63		Crippen Method
logp	0.792		Crippen Method
mcvol	88.560	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
rinpol	802.00		NIST Webbook
tb	437.86	K	Joback Method
tc	632.31	K	Joback Method
tf	218.33	K	Joback Method
vc	0.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.10	J/mol×K	437.86	Joback Method
cpg	181.16	J/mol×K	470.27	Joback Method
cpg	188.95	J/mol×K	502.68	Joback Method
cpg	196.47	J/mol×K	535.08	Joback Method
cpg	203.72	J/mol×K	567.49	Joback Method
cpg	210.69	J/mol×K	599.90	Joback Method
cpg	217.38	J/mol×K	632.31	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=R325385&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