Propanenitrile, 2-methyl-3-(1-methylethyloxy)

Inchi: InChI=1S/C7H13NO/c1-6(2)9-5-7(3)4-8/h6-7H,5H2,1-3H3
InchiKey: XQKSXHAHCPLSIV-UHFFFAOYSA-N
Formula: C7H13NO
SMILES: CC(C#N)COC(C)C
Mol. weight [g/mol]: 127.18

Physical Properties

Property code	Value	Unit	Source
gf	31.36	kJ/mol	Joback Method
hf	-165.71	kJ/mol	Joback Method
hfus	9.53	kJ/mol	Joback Method
hvap	43.29	kJ/mol	Joback Method
log10ws	-1.58		Crippen Method
logp	1.571		Crippen Method
mcvol	116.740	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
rinpol	915.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	915.00		NIST Webbook
tb	483.18	K	Joback Method
tc	677.62	K	Joback Method
tf	225.87	K	Joback Method
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.94	J/mol×K	483.18	Joback Method
cpg	262.91	J/mol×K	515.59	Joback Method
cpg	273.46	J/mol×K	547.99	Joback Method
cpg	283.57	J/mol×K	580.40	Joback Method
cpg	293.25	J/mol×K	612.80	Joback Method
cpg	302.50	J/mol×K	645.21	Joback Method
cpg	311.33	J/mol×K	677.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R130335&Units=SI
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

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