

Propanenitrile, 3-ethoxy-

Other names:	Propionitrile, 3-ethoxy- «beta»-Ethoxypropionitrile 3-Ethoxypropionitrile 3-ethoxypropiononitrile C ₂ H ₅ CH(OC ₂ H ₅)CH ₂ CN
Inchi:	InChI=1S/C ₅ H ₉ NO/c1-2-7-5-3-4-6/h2-3,5H ₂ ,1H ₃
InchiKey:	DCWQZPJHHVLHSV-UHFFFAOYSA-N
Formula:	C ₅ H ₉ NO
SMILES:	CCOCCC#N
Mol. weight [g/mol]:	99.13
CAS:	2141-62-0

Physical Properties

Property code	Value	Unit	Source
affp	807.20	kJ/mol	NIST Webbook
basg	776.50	kJ/mol	NIST Webbook
gf	19.40	kJ/mol	Joback Method
hf	-113.87	kJ/mol	Joback Method
hfus	11.40	kJ/mol	Joback Method
hvap	39.61	kJ/mol	Joback Method
log10ws	-0.87		Crippen Method
logp	0.937		Crippen Method
mvol	88.560	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
tb	444.20	K	NIST Webbook
tc	628.32	K	Joback Method
tf	233.33	K	Joback Method
tt	234.80 ± 0.20	K	NIST Webbook
vc	0.359	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.95	J/mol×K	438.30	Joback Method

cpg	180.74	J/mol×K	469.97	Joback Method
cpg	188.29	J/mol×K	501.64	Joback Method
cpg	195.58	J/mol×K	533.31	Joback Method
cpg	202.62	J/mol×K	564.98	Joback Method
cpg	209.40	J/mol×K	596.65	Joback Method
cpg	215.92	J/mol×K	628.32	Joback Method

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=C2141620&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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