

Crotonamide, 2-cyano-3-(ethoxy)thio-

Inchi:	InChI=1S/C7H10N2OS/c1-3-10-5(2)6(4-8)7(9)11/h3H2,1-2H3,(H2,9,11)/b6-5+
InchiKey:	QRQWVBSLABMWFN-AATRIKPKSA-N
Formula:	C7H10N2OS
SMILES:	CCOC(C)=C(C#N)C(N)=S
Mol. weight [g/mol]:	170.23
CAS:	89943-20-4

Physical Properties

Property code	Value	Unit	Source
gf	282.87	kJ/mol	Joback Method
hf	122.78	kJ/mol	Joback Method
hfus	23.96	kJ/mol	Joback Method
hvap	61.55	kJ/mol	Joback Method
log10ws	-2.34		Crippen Method
logp	1.107		Crippen Method
mcvol	134.470	ml/mol	McGowan Method
pc	3376.28	kPa	Joback Method
tb	630.55	K	Joback Method
tc	865.92	K	Joback Method
tf	340.40	K	Joback Method
vc	0.518	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.43	J/mol×K	630.55	Joback Method
cpg	316.51	J/mol×K	669.78	Joback Method
cpg	324.98	J/mol×K	709.01	Joback Method
cpg	332.90	J/mol×K	748.24	Joback Method
cpg	340.35	J/mol×K	787.47	Joback Method
cpg	347.39	J/mol×K	826.70	Joback Method
cpg	354.07	J/mol×K	865.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C89943204&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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