2-Butenoic acid, 3-(methylamino)-, ethyl ester

Other names:	Crotonic acid, 3-(methylamino)-, ethyl ester
	Ethyl «beta»-(methylamino)crotonate
	Ethyl 3-(methylamino)-2-butenoate
	Ethyl 3-(methylamino)crotonate
Inchi:	InChI=1S/C7H13NO2/c1-4-10-7(9)5-6(2)8-3/h5,8H,4H2,1-3H3/b6-5+
InchiKey:	FARYTWBWLZAXNK-AATRIKPKSA-N
Formula:	C7H13NO2
SMILES:	CCOC(=O)C=C(C)NC
Mol. weight [g/mol]:	143.18
CAS:	870-85-9

Physical Properties

Property code	Value	Unit	Source
gf	-64.80	kJ/mol	Joback Method
hf	-271.71	kJ/mol	Joback Method
hfus	20.66	kJ/mol	Joback Method
hvap	46.81	kJ/mol	Joback Method
log10ws	-1.15		Crippen Method
logp	0.673		Crippen Method
mcvol	122.610	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
tb	490.06	K	Joback Method
tc	681.38	K	Joback Method
tf	274.43	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.54	J/mol×K	490.06	Joback Method
cpg	277.01	J/mol×K	521.95	Joback Method
cpg	287.96	J/mol×K	553.83	Joback Method
cpg	298.40	J/mol×K	585.72	Joback Method
cpg	308.35	J/mol×K	617.61	Joback Method

cpg	317.82	J/mol×K	649.50	Joback Method
cpg	326.82	J/mol×K	681.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C870859&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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