

Ethyl 3-ethoxy-cis-crotonate

Other names:	Ethyl (2Z)-3-ethoxy-2-butenate 2-Butenoic acid, 3-ethoxy-, ethyl ester, (2Z)- Ethyl-3-ethoxy crotonate
Inchi:	InChI=1S/C8H14O3/c1-4-10-7(3)6-8(9)11-5-2/h6H,4-5H2,1-3H3/b7-6+
InchiKey:	ZOCYCSPSSNMXBU-VOTSOKGWSA-N
Formula:	C8H14O3
SMILES:	CCOC(=O)C=C(C)OCC
Mol. weight [g/mol]:	158.19
CAS:	5331-73-7

Physical Properties

Property code	Value	Unit	Source
gf	-250.77	kJ/mol	Joback Method
hf	-478.04	kJ/mol	Joback Method
hfus	19.34	kJ/mol	Joback Method
hvap	45.01	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.490		Crippen Method
mcvol	132.590	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
tb	485.19	K	Joback Method
tc	671.03	K	Joback Method
tf	255.27	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.67	J/molxK	485.19	Joback Method
cpg	298.54	J/molxK	516.16	Joback Method
cpg	309.96	J/molxK	547.14	Joback Method
cpg	320.93	J/molxK	578.11	Joback Method
cpg	331.46	J/molxK	609.09	Joback Method
cpg	341.54	J/molxK	640.06	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C5331737&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
mccvol:	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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