Propanoic acid, 2-mercapto-, ethyl ester

Other names:	Propionic acid, 2-mercapto-, ethyl ester
	Ethyl 2-mercaptopropionate
	Ethyl 2-thiolpropanoate
	Ethyl 2-sulfanylpropanoate
	2-Mercaptopropionic acid, ethyl ester
	Ethyl 2-mercaptopropanoate
Inchi:	InChI=1S/C5H10O2S/c1-3-7-5(6)4(2)8/h4,8H,3H2,1-2H3
InchiKey:	LXXNWCFBZHKFPT-UHFFFAOYSA-N
Formula:	C5H10O2S
SMILES:	CCOC(=O)C(C)S
Mol. weight [g/mol]:	134.20
CAS:	19788-49-9

Physical Properties

Property code	Value	Unit	Source
gf	-215.75	kJ/mol	Joback Method
hf	-358.13	kJ/mol	Joback Method
hfus	12.01	kJ/mol	Joback Method
hvap	42.23	kJ/mol	Joback Method
log10ws	-0.96		Crippen Method
logp	0.868		Crippen Method
mcvol	105.100	ml/mol	McGowan Method
pc	4005.77	kPa	Joback Method
rinpol	901.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	901.00		NIST Webbook
rinpol	925.00		NIST Webbook
ripol	1339.00		NIST Webbook
ripol	1300.00		NIST Webbook
ripol	1339.00		NIST Webbook
ripol	1300.00		NIST Webbook
tb	452.51	K	Joback Method
tc	659.24	K	Joback Method
tf	239.73	K	Joback Method
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.37	J/mol×K	452.51	Joback Method
cpg	213.97	J/mol×K	486.96	Joback Method
cpg	223.19	J/mol×K	521.42	Joback Method
cpg	232.03	J/mol×K	555.87	Joback Method
cpg	240.48	J/mol×K	590.33	Joback Method
cpg	248.55	J/mol×K	624.78	Joback Method
cpg	256.23	J/mol×K	659.24	Joback Method

Sources

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=C19788499&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume