3-(Methylthio)propanoic acid ethyl ester

Other names:	Ethyl 3-(methylthio)propionate
	Propanoic acid, 3-(methylthio)-, ethyl ester
	Ethyl «beta»-methylthiopropionate
	Propionic acid, 3-(methylthio)-, ethyl ester
	3-(Methylthio)propionic acid ethylester
	Ethyl methylthiopropanoate
	Ethyl 3-(methylsulfanyl)propanoate
	Ethyl 3-methylthiopropanoate
Inchi:	InChI=1S/C6H12O2S/c1-3-8-6(7)4-5-9-2/h3-5H2,1-2H3
InchiKey:	YSNWHRKJEKWJNY-UHFFFAOYSA-N
Formula:	C6H12O2S
SMILES:	CCOC(=O)CCSC
Mol. weight [g/mol]:	148.22
CAS:	13327-56-5

Physical Properties

Property code	Value	Unit	Source
gf	-201.16	kJ/mol	Joback Method
hf	-370.10	kJ/mol	Joback Method
hfus	18.21	kJ/mol	Joback Method
hvap	44.92	kJ/mol	Joback Method
log10ws	-1.08		Crippen Method
logp	1.303		Crippen Method
mcvol	119.190	ml/mol	McGowan Method
pc	3337.38	kPa	Joback Method
rinpol	1094.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1071.00		NIST Webbook

rinpol	1078.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1069.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1098.00		NIST Webbook
ripol	1560.00		NIST Webbook
ripol	1560.00		NIST Webbook
ripol	1562.00		NIST Webbook
ripol	1565.00		NIST Webbook
ripol	1581.00		NIST Webbook
ripol	1560.00		NIST Webbook
ripol	1565.00		NIST Webbook
ripol	1561.00		NIST Webbook
ripol	1550.00		NIST Webbook
ripol	1558.00		NIST Webbook
ripol	1557.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1577.00		NIST Webbook
ripol	1562.00		NIST Webbook
ripol	1558.00		NIST Webbook
ripol	1569.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1562.00		NIST Webbook
ripol	1569.00		NIST Webbook
ripol	1580.00		NIST Webbook
ripol	1571.00		NIST Webbook
ripol	1580.00		NIST Webbook
ripol	1560.00		NIST Webbook
ripol	1551.00		NIST Webbook
ripol	1561.00		NIST Webbook
tb	481.75	K	Joback Method
tc	681.10	K	Joback Method
tf	263.94	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	245.41	J/mol×K	481.75	Joback Method
cpg	256.09	J/mol×K	514.98	Joback Method
cpg	266.37	J/mol×K	548.20	Joback Method
cpg	276.25	J/mol×K	581.43	Joback Method
cpg	285.71	J/mol×K	614.65	Joback Method
cpg	294.75	J/mol×K	647.88	Joback Method
cpg	303.37	J/mol×K	681.10	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=C13327565&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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