Thiopropionic acid, S-ethyl ester

Other names:	Ethyl thiopropionate
	Propanethioic acid, S-ethyl ester
	Thiopropionic acid, S-ethyl ester
	S-ethyl propanethioate
Inchi:	InChI=1S/C5H10OS/c1-3-5(6)7-4-2/h3-4H2,1-2H3
InchiKey:	HNEVHBHRLCAKKQ-UHFFFAOYSA-N
Formula:	C5H10OS
SMILES:	CCSC(=O)CC
Mol. weight [g/mol]:	118.20

Physical Properties

Property code	Value	Unit	Source
hf	-251.78	kJ/mol	Cheméo Relay (1.0)
hfus	14.44	kJ/mol	Joback Method
hvap	40.25	kJ/mol	Cheméo Relay (1.0)
ie	9.13	eV	Cheméo Relay (1.0)
log10ws	-1.23		Cheméo Relay (1.0)
logp	1.676		Crippen Method
mcvol	99.230	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
rinpol	846.00		NIST Webbook
rinpol	872.90		NIST Webbook
rinpol	849.00		NIST Webbook
rinpol	849.00		NIST Webbook
tb	410.74	K	Cheméo Relay (1.0)
tc	597.20	K	Cheméo Relay (1.0)
tf	238.97	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.53	J/mol×K	436.45	Joback Method
cpg	194.04	J/mol×K	470.30	Joback Method
cpg	203.15	J/mol×K	504.16	Joback Method

cpg	211.86	J/mol×K	538.01	Joback Method
cpg	220.19	J/mol×K	571.86	Joback Method
cpg	228.12	J/mol×K	605.72	Joback Method
cpg	235.68	J/mol×K	639.57	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2432420&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point