Carbonodithioic acid, O,S-diethyl ester

Other names:	Carbonic acid, dithio-, O,S-diethyl ester
	Diethyl xanthate
	Ethyl O-ethylxanthate
	Ethyl S-ethyl xanthate
	O,S-Diethyl dithiocarbonate
	Ethyl-ethylxanthate
Inchi:	InChI=1S/C5H10OS2/c1-3-6-5(7)8-4-2/h3-4H2,1-2H3
InchiKey:	JGZZEAPGGFAOAY-UHFFFAOYSA-N
Formula:	C5H10OS2
SMILES:	CCOC(=S)SCC
Mol. weight [g/mol]:	150.26
CAS:	623-79-0

Physical Properties

Property code	Value	Unit	Source
gf	36.40	kJ/mol	Joback Method
hf	-90.38	kJ/mol	Joback Method
hfus	18.63	kJ/mol	Joback Method
hvap	42.68	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	2.061		Crippen Method
mcvol	115.580	ml/mol	McGowan Method
pc	3877.12	kPa	Joback Method
tb	475.04	K	Joback Method
tc	694.34	K	Joback Method
tf	237.01	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.81	J/mol×K	475.04	Joback Method
cpg	229.54	J/mol×K	511.59	Joback Method
cpg	238.73	J/mol×K	548.14	Joback Method

cpg	247.42	J/mol×K	584.69	Joback Method
cpg	255.63	J/mol×K	621.24	Joback Method
cpg	263.37	J/mol×K	657.79	Joback Method
cpg	270.67	J/mol×K	694.34	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=C623790&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume