Methyl trichlorothioacrylate

Inchi: InChI=1S/C4H3Cl3OS/c1-8-4(9)2(5)3(6)7/h1H3
InchiKey: WUEKZQWKWJIUPB-UHFFFAOYSA-N
Formula: C4H3Cl3OS
SMILES: COC(=S)C(Cl)=C(Cl)Cl
Mol. weight [g/mol]: 205.49
CAS: 76619-91-5

Physical Properties

Property code	Value	Unit	Source
gf	22.19	kJ/mol	Joback Method
hf	-61.19	kJ/mol	Joback Method
hfus	22.08	kJ/mol	Joback Method
hvap	46.91	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.846		Crippen Method
mcvol	117.560	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
sl	324.30	J/mol×K	NIST Webbook
tb	499.59	K	Joback Method
tc	737.29	K	Joback Method
tf	248.10	K	Joback Method
tt	286.25 ± 0.02	K	NIST Webbook
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.38	J/mol×K	618.44	Joback Method
cpg	205.53	J/mol×K	658.06	Joback Method
cpg	209.31	J/mol×K	697.67	Joback Method
cpg	186.13	J/mol×K	499.59	Joback Method
cpg	191.74	J/mol×K	539.21	Joback Method
cpg	196.80	J/mol×K	578.82	Joback Method
cpg	212.80	J/mol×K	737.29	Joback Method

cpl	244.90	J/mol×K	298.15	NIST Webbook
hfust	20.37	kJ/mol	286.25	NIST Webbook
hvapt	64.80	kJ/mol	403.00	NIST Webbook
sfust	71.20	J/mol×K	286.25	NIST Webbook

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=C76619915&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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