Sulfurous acid, dipropyl ester

Other names:	Di-n-propyl sulphite
	Dipropyl ester of sulfurous acid
	Dipropyl sulfite
	Dipropyl sulphite
	Sulphurous acid dipropyl ester
	di-n-Propyl sulfite
Inchi:	InChI=1S/C6H14O3S/c1-3-5-8-10(7)9-6-4-2/h3-6H2,1-2H3
InchiKey:	MAIQPVFXODAAIG-UHFFFAOYSA-N
Formula:	C6H14O3S
SMILES:	CCCOS(=O)OCCC
Mol. weight [g/mol]:	166.24
CAS:	623-98-3

Physical Properties

Property code	Value	Unit	Source
chl	-4317.30 ± 1.00	kJ/mol	NIST Webbook
gf	-428.07	kJ/mol	Joback Method
hf	-588.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-646.60 ± 1.10	kJ/mol	NIST Webbook
hfus	21.43	kJ/mol	Joback Method
hvap	59.00 ± 2.00	kJ/mol	NIST Webbook
log10ws	-1.12		Crippen Method
logp	1.418		Crippen Method
mcvol	129.360	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
tb	465.00 ± 1.00	K	NIST Webbook
tb	464.00 ± 3.00	K	NIST Webbook
tc	615.01	K	Joback Method
tf	238.32	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	264.37	J/mol×K	439.80	Joback Method
cpg	275.39	J/mol×K	469.00	Joback Method
cpg	286.14	J/mol×K	498.20	Joback Method
cpg	296.60	J/mol×K	527.41	Joback Method
cpg	306.76	J/mol×K	556.61	Joback Method
cpg	316.60	J/mol×K	585.81	Joback Method
cpg	326.11	J/mol×K	615.01	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.30165e+01
Coeff. B	-3.31458e+03
Coeff. C	-7.03230e+01
Temperature range (K), min.	330.72
Temperature range (K), max.	500.51

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C623983&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

Legend

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfl: Liquid phase 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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume