Propane, 1,1'-sulfonylbis-

Other names:	1,1'-SULPHONYLBISPROPANE
	DIPROPYL SULFONE
	Di-n-propyl sulfone
	Dipropyl sulphone
	Propyl sulfone
	n-Propyl sulfone
Inchi:	InChI=1S/C6H14O2S/c1-3-5-9(7,8)6-4-2/h3-6H2,1-2H3
InchiKey:	JEXYCADTAFPULN-UHFFFAOYSA-N
Formula:	C6H14O2S
SMILES:	CCCS(=O)(=O)CCC
Mol. weight [g/mol]:	150.24
CAS:	598-03-8

Physical Properties

Property code	Value	Unit	Source
chl	-4416.00 ± 0.63	kJ/mol	NIST Webbook
gf	-468.90	kJ/mol	Joback Method
hf	-468.30 ± 2.60	kJ/mol	NIST Webbook
hfl	-548.19 ± 0.84	kJ/mol	NIST Webbook
hfus	22.67	kJ/mol	Joback Method
hvap	80.00 ± 2.00	kJ/mol	NIST Webbook
log10ws	-1.17		Crippen Method
logp	1.221		Crippen Method
mcvol	123.490	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
tb	542.00 ± 3.00	K	NIST Webbook
tc	547.33	K	Joback Method
tf	195.94	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.01	J/mol×K	384.46	Joback Method

cpg	240.33	J/mol×K	411.61	Joback Method
cpg	251.31	J/mol×K	438.75	Joback Method
cpg	261.93	J/mol×K	465.90	Joback Method
cpg	272.19	J/mol×K	493.04	Joback Method
cpg	282.10	J/mol×K	520.19	Joback Method
cpg	291.65	J/mol×K	547.33	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49813e+01
Coeff. B	-4.66224e+03
Coeff. C	-9.21040e+01
Temperature range (K), min.	409.40
Temperature range (K), max.	574.25

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.02832e+02
Coeff. B	-1.22739e+04
Coeff. C	-1.21800e+01
Coeff. D	3.66502e-06
Temperature range (K), min.	303.00
Temperature range (K), max.	763.00

Sources

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1889.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C598038&Units=SI

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

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