

Propane, 1,1'-sulfinylbis-

Other names:	(n-C3H7)2SO 1,1'-Sulphinylbispropane 1,1'-sulfinylbispropane Di-n-propyl sulfoxid Di-n-propyl sulphoxide Di-n-propylsulfoxide Dipropyl sulphoxide NSC 75838 Sulfoxide, dipropyl di-n-propyl sulfoxide dipropyl sulfoxide propyl sulfoxide
Inchi:	InChI=1S/C6H14OS/c1-3-5-8(7)6-4-2/h3-6H2,1-2H3
InchiKey:	BQCCJWMQESHLIT-UHFFFAOYSA-N
Formula:	C6H14OS
SMILES:	CCCS(=O)CCC
Mol. weight [g/mol]:	134.24

Physical Properties

Property code	Value	Unit	Source
chl	-4634.60 ± 0.40	kJ/mol	NIST Webbook
hf	-255.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-329.00 ± 0.80	kJ/mol	NIST Webbook
hfus	19.05	kJ/mol	Joback Method
hvap	74.00 ± 1.00	kJ/mol	NIST Webbook
ie	8.60	eV	NIST Webbook
log10ws	-0.86		Cheméo Relay (1.0)
logp	1.555		Crippen Method
mcvol	117.620	ml/mol	McGowan Method
tb	475.00 ± 1.00	K	NIST Webbook
tf	297.90 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.98	J/mol×K	394.96	Joback Method
cpg	229.40	J/mol×K	424.18	Joback Method
cpg	240.43	J/mol×K	453.41	Joback Method
cpg	251.06	J/mol×K	482.63	Joback Method
cpg	261.30	J/mol×K	511.85	Joback Method
cpg	271.16	J/mol×K	541.08	Joback Method
cpg	280.63	J/mol×K	570.30	Joback Method
srf	0.03	N/m	298.15	Surface and bulk behavior of (dialkylsulfoxides + carbon tetrachloride) mixtures
srf	0.03	N/m	303.15	Surface and bulk behavior of (dialkylsulfoxides + carbon tetrachloride) mixtures
srf	0.03	N/m	308.15	Surface and bulk behavior of (dialkylsulfoxides + carbon tetrachloride) mixtures
srf	0.03	N/m	313.15	Surface and bulk behavior of (dialkylsulfoxides + carbon tetrachloride) mixtures
srf	0.03	N/m	298.15	Surface Tension and Refractive Index of Dialkylsulfoxide + Water Mixtures at Several Temperatures
srf	0.03	N/m	303.15	Surface Tension and Refractive Index of Dialkylsulfoxide + Water Mixtures at Several Temperatures
srf	0.03	N/m	308.15	Surface Tension and Refractive Index of Dialkylsulfoxide + Water Mixtures at Several Temperatures

srf	0.03	N/m	313.15	Surface Tension and Refractive Index of Dialkylsulfoxide + Water Mixtures at Several Temperatures
srf	0.03	N/m	318.15	Surface Tension and Refractive Index of Dialkylsulfoxide + Water Mixtures at Several Temperatures
srf	0.03	N/m	323.15	Surface Tension and Refractive Index of Dialkylsulfoxide + Water Mixtures at Several Temperatures
srf	0.03	N/m	328.15	Surface Tension and Refractive Index of Dialkylsulfoxide + Water Mixtures at Several Temperatures

Sources

Cheméo Relay (1.0, beta):

Surface and bulk behavior of (dialkylsulfoxides + carbon tetrachloride) mixtures:

<https://www.doi.org/10.1016/j.jct.2009.06.021>

Crippen Method:

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

Surface Tension and Refractive Index of Dialkylsulfoxide + Water Mixtures at Several Temperatures:

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

NIST Webbook:

<https://www.doi.org/10.1021/je7001013>

Crippen Method:

<http://link.springer.com/article/10.1007/BF02311772>

Cheméo Relay (1.0):

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C4253912&Units=SI>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
srf:	Surface Tension
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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