Diisobutyl sulfone

Other names:	(iso-C4H9)2SO2
	1,1'-Sulphonylbis(2-methyl-propane)
	Diisobutyl sulphone
	Isobutyl sulfone
	Propane, 1,1'-sulfonylbis*2-methyl-
	Propane, 1,1'-sulfonylbis[2-methyl-
Inchi:	InChI=1S/C8H18O2S/c1-7(2)5-11(9,10)6-8(3)4/h7-8H,5-6H2,1-4H3
InchiKey:	ULSLZZKKTPQNNJ-UHFFFAOYSA-N
Formula:	C8H18O2S
SMILES:	CC(C)CS(=O)(=O)CC(C)C
Mol. weight [g/mol]:	178.29
CAS:	10495-45-1

Physical Properties

Property code	Value	Unit	Source
chl	-5697.69 ± 0.59	kJ/mol	NIST Webbook
gf	-456.94	kJ/mol	Joback Method
hf	-535.60 ± 2.60	kJ/mol	NIST Webbook
hfl	-625.17 ± 0.84	kJ/mol	NIST Webbook
hfus	20.81	kJ/mol	Joback Method
hvap	90.00 ± 3.00	kJ/mol	NIST Webbook
ie	9.54 ± 0.05	eV	NIST Webbook
log10ws	-1.52		Crippen Method
logp	1.713		Crippen Method
mcvol	151.670	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
tb	374.00 ± 3.00	K	NIST Webbook
tb	538.00	K	NIST Webbook
tc	598.32	K	Joback Method
tf	290.00	K	NIST Webbook
tf	290.10 ± 0.60	K	NIST Webbook
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.59	J/mol×K	429.34	Joback Method
cpg	323.91	J/mol×K	457.50	Joback Method
cpg	337.72	J/mol×K	485.67	Joback Method
cpg	351.02	J/mol×K	513.83	Joback Method
cpg	363.80	J/mol×K	541.99	Joback Method
cpg	376.08	J/mol×K	570.15	Joback Method
cpg	387.85	J/mol×K	598.32	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49079e+01
Coeff. B	-4.60194e+03
Coeff. C	-9.07560e+01
Temperature range (K), min.	405.52
Temperature range (K), max.	570.30

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10495451&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

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

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
ie:	Ionization energy
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