Sulfurous acid, dibutyl ester

Other names:	Butyl sulfite (Bu2SO3)
	Di-n-butyl sulphite
	Dibutyl sulfite
	Dibutyl sulphite
	Sulphurous acid dibutyl ester
Inchi:	InChI=1S/C8H18O3S/c1-3-5-7-10-12(9)11-8-6-4-2/h3-8H2,1-2H3
InchiKey:	FEYYOXFAQQJEIG-UHFFFAOYSA-N
Formula:	C8H18O3S
SMILES:	CCCCOS(=O)OCCCC
Mol. weight [g/mol]:	194.29
CAS:	626-85-7

Physical Properties

Property code	Value	Unit	Source
chl	-5629.80 ± 1.90	kJ/mol	NIST Webbook
gf	-411.23	kJ/mol	Joback Method
hf	-625.10 ± 5.00	kJ/mol	NIST Webbook
hfl	-692.90 ± 4.20	kJ/mol	NIST Webbook
hfus	26.61	kJ/mol	Joback Method
hvap	68.00 ± 2.00	kJ/mol	NIST Webbook
log10ws	-1.96		Crippen Method
logp	2.199		Crippen Method
mcvol	157.540	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
tb	485.56	K	Joback Method
tc	658.13	K	Joback Method
tf	260.86	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.03	J/mol×K	485.56	Joback Method
cpg	362.31	J/mol×K	514.32	Joback Method

cpg	375.18	J/mol×K	543.08	Joback Method
cpg	387.64	J/mol×K	571.84	Joback Method
cpg	399.67	J/mol×K	600.61	Joback Method
cpg	411.26	J/mol×K	629.37	Joback Method
cpg	422.40	J/mol×K	658.13	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.25901e+01
Coeff. B	-3.45077e+03
Coeff. C	-8.10260e+01
Temperature range (K), min.	361.52
Temperature range (K), max.	555.12

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C626857&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