Butane, 1,1'-sulfonylbis-

Other names:	1,1'-SULPHONYLBISBUTANE
	1-(Butylsulfonyl)butane
	Butyl sulfone
	DIBUTYL SULFONE
	Di-n-butyl sulfone
	Dibutyl sulphone
	NSC 2116
	n-Butyl sulfone
Inchi:	InChI=1S/C8H18O2S/c1-3-5-7-11(9,10)8-6-4-2/h3-8H2,1-2H3
InchiKey:	AIDFJGKWTOULTC-UHFFFAOYSA-N
Formula:	C8H18O2S
SMILES:	CCCCS(=O)(=O)CCCC
Mol. weight [g/mol]:	178.29
CAS:	598-04-9

Physical Properties

Property code	Value	Unit	Source
chs	-5712.70 ± 1.90	kJ/mol	NIST Webbook
gf	-452.06	kJ/mol	Joback Method
hf	-509.80 ± 3.20	kJ/mol	NIST Webbook
hfs	-610.20 ± 2.00	kJ/mol	NIST Webbook
hfus	27.85	kJ/mol	Joback Method
hsub	100.00 ± 2.00	kJ/mol	NIST Webbook
hvap	52.04	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	2.001		Crippen Method
mcvol	151.670	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
tb	430.22	K	Joback Method
tc	592.13	K	Joback Method
tf	218.48	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.58	J/mol×K	430.22	Joback Method
cpg	323.15	J/mol×K	457.20	Joback Method
cpg	336.26	J/mol×K	484.19	Joback Method
cpg	348.90	J/mol×K	511.17	Joback Method
cpg	361.09	J/mol×K	538.16	Joback Method
cpg	372.83	J/mol×K	565.14	Joback Method
cpg	384.11	J/mol×K	592.13	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.36446e+01
Coeff. B	-4.38453e+03
Coeff. C	-9.79420e+01
Temperature range (K), min.	426.20
Temperature range (K), max.	624.10

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.17265e+02
Coeff. B	-1.37461e+04
Coeff. C	-1.41440e+01
Coeff. D	4.13287e-06
Temperature range (K), min.	318.00
Temperature range (K), max.	767.00

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol1891.mol

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C598049&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1891
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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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