1-Butanesulfonyl chloride

Other names:	1-Butylsulfonyl chloride
	Butane-1-sulfonyl chloride
	Butanesulfonyl chloride
	Butylsulfonyl chloride
	butane-1-sulphonyl chloride
Inchi:	InChI=1S/C4H9ClO2S/c1-2-3-4-8(5,6)7/h2-4H2,1H3
InchiKey:	WEDIIKBPDQQQJU-UHFFFAOYSA-N
Formula:	C4H9ClO2S
SMILES:	CCCCS(=O)(=O)Cl
Mol. weight [g/mol]:	156.63
CAS:	2386-60-9

Physical Properties

Property code	Value	Unit	Source
gf	-497.67	kJ/mol	Joback Method
hf	-594.98	kJ/mol	Joback Method
hfus	21.69	kJ/mol	Joback Method
hvap	55.70	kJ/mol	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.355		Crippen Method
mcvol	107.550	ml/mol	McGowan Method
pc	4540.80	kPa	Joback Method
tb	376.13	K	Joback Method
tc	547.73	K	Joback Method
tf	203.32	K	Joback Method
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.61	J/mol×K	490.53	Joback Method
cpg	223.07	J/mol×K	519.13	Joback Method
cpg	182.97	J/mol×K	376.13	Joback Method
cpg	191.55	J/mol×K	404.73	Joback Method

cpg	199.85	J/mol×K	433.33	Joback Method
cpg	207.88	J/mol×K	461.93	Joback Method
cpg	230.23	J/mol×K	547.73	Joback Method
hvapt	52.90	kJ/mol	423.50	NIST Webbook
hvapt	60.20	kJ/mol	268.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57348e+01
Coeff. B	-4.60475e+03
Coeff. C	-5.79430e+01
Temperature range (K), min.	356.04
Temperature range (K), max.	499.72

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2386609&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

Legend

cpg: Ideal gas heat capacity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions

hvapt: Enthalpy of vaporization at a given temperature

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