

Sulphuric acid dibutyl ester

Other names:	Dibutyl sulphate Sulfuric acid, dibutyl ester Di-n-butylsulfat Dibutylsulfate Di-n-butyl sulphate
Inchi:	InChI=1S/C8H18O4S/c1-3-5-7-11-13(9,10)12-8-6-4-2/h3-8H2,1-2H3
InchiKey:	LMEDOLJKVASKTP-UHFFFAOYSA-N
Formula:	C8H18O4S
SMILES:	CCCCOS(=O)(=O)OCCCC
Mol. weight [g/mol]:	210.29
CAS:	625-22-9

Physical Properties

Property code	Value	Unit	Source
chl	-5418.20 ± 7.10	kJ/mol	NIST Webbook
gf	-662.06	kJ/mol	Joback Method
hf	-829.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-904.40 ± 2.60	kJ/mol	NIST Webbook
hfus	30.23	kJ/mol	Joback Method
hvap	76.00 ± 2.00	kJ/mol	NIST Webbook
log10ws	-2.16		Crippen Method
logp	1.865		Crippen Method
mcvol	163.410	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
tb	475.06	K	Joback Method
tc	637.13	K	Joback Method
tf	193.50 ± 0.50	K	NIST Webbook
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.18	J/mol×K	475.06	Joback Method
cpg	374.32	J/mol×K	502.07	Joback Method

cpg	387.08	J/mol×K	529.08	Joback Method
cpg	399.46	J/mol×K	556.10	Joback Method
cpg	411.44	J/mol×K	583.11	Joback Method
cpg	423.01	J/mol×K	610.12	Joback Method
cpg	434.17	J/mol×K	637.13	Joback Method

Sources

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=C625229&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/48-433-8/Sulphuric-acid-dibutyl-ester.pdf>

Generated by Cheméo on 2025-12-05 20:35:35.040565557 +0000 UTC m=+4715132.570606217.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.