Disulfide, dibutyl

Other names:	(n-C4H9S)2
	5,6-Dithiadecane
	Butyl disulfide
	Di-n-butyl disulfide
	Dibutyl disulfide
	Dibutyl disulphide
	NSC 36626
	n-Butyl disulfide
Inchi:	InChI=1S/C8H18S2/c1-3-5-7-9-10-8-6-4-2/h3-8H2,1-2H3
InchiKey:	CUDSBWGCGSUXDB-UHFFFAOYSA-N
Formula:	C8H18S2
SMILES:	CCCCSSCCCC
Mol. weight [g/mol]:	178.36
CAS:	629-45-8

Physical Properties

Property code	Value	Unit	Source
chl	-6702.30 ± 1.80	kJ/mol	NIST Webbook
gf	82.72	kJ/mol	Joback Method
hf	-158.40 ± 2.60	kJ/mol	NIST Webbook
hfl	-222.90 ± 2.00	kJ/mol	NIST Webbook
hfus	24.74	kJ/mol	Joback Method
hvap	64.50	kJ/mol	NIST Webbook
hvap	64.10	kJ/mol	NIST Webbook
hvap	65.00 ± 2.00	kJ/mol	NIST Webbook
hvap	62.27	kJ/mol	NIST Webbook
hvap	62.30	kJ/mol	NIST Webbook
hvap	62.30 ± 0.20	kJ/mol	NIST Webbook
ie	8.51	eV	NIST Webbook
log10ws	-3.93		Crippen Method
logp	3.968		Crippen Method
mcvol	156.280	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
rinpol	1298.20		NIST Webbook
rinpol	1307.20		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1288.00		NIST Webbook

rinpol	1289.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1293.00		NIST Webbook
ripol	1567.00		NIST Webbook
ripol	1592.00		NIST Webbook
ripol	1580.00		NIST Webbook
ripol	1568.00		NIST Webbook
tb	504.20	K	NIST Webbook
tc	726.00	K	Joback Method
tf	248.72	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.03	J/mol×K	588.67	Joback Method
cpg	382.19	J/mol×K	623.00	Joback Method
cpg	394.70	J/mol×K	657.33	Joback Method
cpg	406.56	J/mol×K	691.67	Joback Method
cpg	340.73	J/mol×K	520.00	Joback Method
cpg	355.21	J/mol×K	554.33	Joback Method
cpg	417.78	J/mol×K	726.00	Joback Method
pvap	90.32	kPa	504.20	Critical Point and Vapor Pressure Measurements for 17 Compounds by a Low Residence Time Flow Method
pvap	180.30	kPa	535.70	Critical Point and Vapor Pressure Measurements for 17 Compounds by a Low Residence Time Flow Method

pvap	349.60	kPa	571.70	Critical Point and Vapor Pressure Measurements for 17 Compounds by a Low Residence Time Flow Method
pvap	695.70	kPa	614.90	Critical Point and Vapor Pressure Measurements for 17 Compounds by a Low Residence Time Flow Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49124e+01
Coeff. B	-4.35271e+03
Coeff. C	-8.13620e+01
Temperature range (K), min.	378.99
Temperature range (K), max.	534.73

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=C629458&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
Critical Point and Vapor Pressure Measurements for 17 Compounds by a Low Residence Time Flow Method:	https://www.doi.org/10.1021/je060269j

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume