

ETHYL N-BUTYL DISULPHIDE

Other names:	3,4-Dithiaoctane Butyl ethyl disulfide Disulfide, butyl ethyl Ethyl n-butyl disulfide
Inchi:	InChI=1S/C6H14S2/c1-3-5-6-8-7-4-2/h3-6H2,1-2H3
InchiKey:	QEYJAENSRLNDFW-UHFFFAOYSA-N
Formula:	C6H14S2
SMILES:	CCCCSSCC
Mol. weight [g/mol]:	150.31
CAS:	63986-03-8

Physical Properties

Property code	Value	Unit	Source
hf	-105.21	kJ/mol	Cheméo Relay (1.0)
hfus	19.56	kJ/mol	Joback Method
hvap	53.48	kJ/mol	Cheméo Relay (1.0)
ie	8.44	eV	Cheméo Relay (1.0)
log10ws	-3.25		Cheméo Relay (1.0)
logp	3.188		Crippen Method
mcvol	128.100	ml/mol	McGowan Method
rinpol	1120.00		NIST Webbook
rinpol	1120.00		NIST Webbook
ripol	1427.00		NIST Webbook
ripol	1427.00		NIST Webbook
tb	466.00 ± 1.70	K	NIST Webbook
tc	664.88	K	Cheméo Relay (1.0)
tf	187.99	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.01	J/mol×K	474.24	Joback Method
cpg	266.31	J/mol×K	509.61	Joback Method
cpg	278.07	J/mol×K	544.98	Joback Method

cpg	289.29	J/mol×K	580.35	Joback Method
cpg	299.98	J/mol×K	615.72	Joback Method
cpg	310.13	J/mol×K	651.09	Joback Method
cpg	319.76	J/mol×K	686.46	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.50291e+01
Coeff. B	-4.09594e+03
Coeff. C	-7.16290e+01
Temperature range (K), min.	349.48
Temperature range (K), max.	493.12

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63986038&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg:	Ideal gas heat capacity
hf:	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
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

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