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
gf	65.88	kJ/mol	Joback Method
hf	-83.43	kJ/mol	Joback Method
hfus	19.56	kJ/mol	Joback Method
hvap	42.58	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	3.188		Crippen Method
mcvol	128.100	ml/mol	McGowan Method
pc	3228.31	kPa	Joback 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	686.46	K	Joback Method
tf	226.18	K	Joback Method
vc	0.479	m3/kmol	Joback Method

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(Pvp) = 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

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

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