Disulfide, butyl pentyl

Other names:	5,6-Dithiaundecane
	Amyl butyl disulfide
	n-Amyl n-butyl disulfide
	n-Butyl n-pentyl disulphide
Inchi:	InChI=1S/C9H20S2/c1-3-5-7-9-11-10-8-6-4-2/h3-9H2,1-2H3
InchiKey:	KIBWKQMJVBZNFS-UHFFFAOYSA-N
Formula:	C9H20S2
SMILES:	CCCCCSSCCCC
Mol. weight [g/mol]:	192.39
CAS:	---

Physical Properties

Property code	Value	Unit	Source
af	0.4803		Cheméo Relay (1.0)
gf	91.14	kJ/mol	Joback Method
hf	-177.33	kJ/mol	Cheméo Relay (1.0)
hfus	27.33	kJ/mol	Joback Method
hvap	67.36	kJ/mol	Cheméo Relay (1.0)
ie	8.30	eV	Cheméo Relay (1.0)
log10ws	-4.80		Cheméo Relay (1.0)
logp	4.358		Crippen Method
mcvol	170.370	ml/mol	McGowan Method
pc	2384.19	kPa	Joback Method
rinpol	1397.00		NIST Webbook
ripol	1690.00		NIST Webbook
tb	519.16	K	Cheméo Relay (1.0)
tc	709.02	K	Cheméo Relay (1.0)
tf	222.01	K	Cheméo Relay (1.0)
vc	0.640	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	386.99	J/mol×K	542.88	Joback Method

cpg	402.36	J/mol×K	576.71	Joback Method
cpg	417.01	J/mol×K	610.53	Joback Method
cpg	430.95	J/mol×K	644.36	Joback Method
cpg	444.19	J/mol×K	678.18	Joback Method
cpg	456.73	J/mol×K	712.01	Joback Method
cpg	468.59	J/mol×K	745.83	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46243e+01
Coeff. B	-4.36146e+03
Coeff. C	-8.56710e+01
Temperature range (K), min.	389.89
Temperature range (K), max.	554.00

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C72437526&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):

Legend

af: Acentric Factor
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
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