Propyl n-butyl disulfide

Other names:	4,5-Dithianonane
	Butyl propyl disulfide
	Disulfide, butyl propyl
	n-Propyl n-butyl disulphide
	propyl butyl disulfide
Inchi:	InChI=1S/C7H16S2/c1-3-5-7-9-8-6-4-2/h3-7H2,1-2H3
InchiKey:	VITWKRWSBFUVDT-UHFFFAOYSA-N
Formula:	C7H16S2
SMILES:	CCCCSSCCC
Mol. weight [g/mol]:	164.33
CAS:	72437-64-0

Physical Properties

Property code	Value	Unit	Source
gf	74.30	kJ/mol	Joback Method
hf	-104.07	kJ/mol	Joback Method
hfus	22.15	kJ/mol	Joback Method
hvap	44.81	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.578		Crippen Method
mcvol	142.190	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
rinpol	1207.00		NIST Webbook
rinpol	1212.00		NIST Webbook
rinpol	1212.00		NIST Webbook
rinpol	1207.00		NIST Webbook
ripol	1515.00		NIST Webbook
ripol	1493.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1493.00		NIST Webbook
ripol	1540.00		NIST Webbook
tb	497.12	K	Joback Method
tc	706.23	K	Joback Method
tf	237.45	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.36	J/mol×K	497.12	Joback Method
cpg	309.83	J/mol×K	531.97	Joback Method
cpg	322.69	J/mol×K	566.82	Joback Method
cpg	334.95	J/mol×K	601.67	Joback Method
cpg	346.61	J/mol×K	636.52	Joback Method
cpg	357.67	J/mol×K	671.38	Joback Method
cpg	368.15	J/mol×K	706.23	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49587e+01
Coeff. B	-4.22036e+03
Coeff. C	-7.68560e+01
Temperature range (K), min.	364.52
Temperature range (K), max.	514.32

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C72437640&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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