

Disulfide, pentyl propyl

Other names:	4,5-Dithiadecane Pentyl propyl disulfide Propyl pentyl disulfide
Inchi:	InChI=1S/C8H18S2/c1-3-5-6-8-10-9-7-4-2/h3-8H2,1-2H3
InchiKey:	XFQOVVIJIMLZCY-UHFFFAOYSA-N
Formula:	C8H18S2
SMILES:	CCCCSSCCC
Mol. weight [g/mol]:	178.36
CAS:	67727-99-5

Physical Properties

Property code	Value	Unit	Source
gf	82.72	kJ/mol	Joback Method
hf	-124.71	kJ/mol	Joback Method
hfus	24.74	kJ/mol	Joback Method
hvap	47.04	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.968		Crippen Method
mcvol	156.280	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
rmpol	1304.00		NIST Webbook
ripol	1568.00		NIST Webbook
tb	520.00	K	Joback Method
tc	726.00	K	Joback Method
tf	248.72	K	Joback Method
vc	0.592	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.73	J/mol×K	520.00	Joback Method
cpg	355.21	J/mol×K	554.33	Joback Method
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	417.78	J/mol×K	726.00	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49392e+01
Coeff. B	-4.35401e+03
Coeff. C	-8.19180e+01
Temperature range (K), min.	379.09
Temperature range (K), max.	534.16

Sources

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=C67727995&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/ci9903071

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

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