Methyl pentyl disulfide

Other names:	2,3-Dithiaoctane
	Amyl methyl disulfide
	Disulfide, methyl pentyl
	Methyl n-amyl disulfide
	Methyl n-pentyl disulphide
Inchi:	InChI=1S/C6H14S2/c1-3-4-5-6-8-7-2/h3-6H2,1-2H3
InchiKey:	VDJXDNLYBDHPHP-UHFFFAOYSA-N
Formula:	C6H14S2
SMILES:	CCCCCSSC
Mol. weight [g/mol]:	150.31
CAS:	72437-68-4

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	1142.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1150.00		NIST Webbook
ripol	1445.00		NIST Webbook
ripol	1445.00		NIST Webbook
ripol	1463.00		NIST Webbook
ripol	1463.00		NIST Webbook
tb	474.24	K	Joback Method
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	1.53867e+01
Coeff. B	-4.22524e+03
Coeff. C	-7.26860e+01
Temperature range (K), min.	352.52
Temperature range (K), max.	492.06

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C72437684&Units=SI

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