2,4-Dithiapentane

Other names:	2,4-Dithiopentane Bis(methylmercapto)methane Bis(methylsulfanyl)methane Bis(methylthio)methane CH3SCH2SCH3 Formaldehyde dimethyl mercaptal Methane, bis(methylthio)- Methylenebis(methyl sulfide) NSC 96010 Thioformaldehyde dimethyl acetal Thioformaldehyde dimethylthioacetal bis(methylthio)methan
Inchi:	InChI=1S/C3H8S2/c1-4-3-5-2/h3H2,1-2H3
InchiKey:	LOCDPORVFVOGCR-UHFFFAOYSA-N
Formula:	C3H8S2
SMILES:	CSCSC
Mol. weight [g/mol]:	108.23
CAS:	1618-26-4

Physical Properties

Property code	Value	Unit	Source
gf	40.62	kJ/mol	Joback Method
hf	-21.51	kJ/mol	Joback Method
hfus	11.79	kJ/mol	Joback Method
hvap	35.91	kJ/mol	Joback Method
ie	8.65	eV	NIST Webbook
ie	8.67	eV	NIST Webbook
log10ws	-1.34		Crippen Method
logp	1.670		Crippen Method
mcvol	85.830	ml/mol	McGowan Method
pc	4615.13	kPa	Joback Method
rinpol	903.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	871.00		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	881.00		NIST Webbook

rinpol	889.00		NIST Webbook
rinpol	873.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	904.00		NIST Webbook
ripol	1300.00		NIST Webbook
ripol	1290.00		NIST Webbook
ripol	1272.00		NIST Webbook
ripol	1285.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1256.00		NIST Webbook
ripol	1256.00		NIST Webbook
ripol	1274.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1289.00		NIST Webbook
ripol	1260.00		NIST Webbook
ripol	1282.00		NIST Webbook
tb	421.20	K	NIST Webbook
tb	415.50 ± 0.50	K	NIST Webbook
tc	626.51	K	Joback Method
tf	192.37	K	Joback Method
vc	0.311	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	140.21	J/mol×K	405.60	Joback Method
cpg	147.98	J/mol×K	442.42	Joback Method
cpg	155.48	J/mol×K	479.24	Joback Method
cpg	162.70	J/mol×K	516.06	Joback Method
cpg	169.63	J/mol×K	552.88	Joback Method
cpg	176.26	J/mol×K	589.70	Joback Method
cpg	182.59	J/mol×K	626.51	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	314.00	K	1.53	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43224e+01
Coeff. B	-3.52228e+03
Coeff. C	-5.82300e+01
Temperature range (K), min.	309.20
Temperature range (K), max.	449.12

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=C1618264&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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