Disulfide, ethyl 1-methylethyl

Other names:	2-Methyl-3,4-dithiahexane
	Disulfide, ethyl isopropyl
	Ethyl 1-methylethyl disulfide
	Ethyl i-propyl disulfide
	Ethyl isopropyl disulfide
Inchi:	InChI=1S/C5H12S2/c1-4-6-7-5(2)3/h5H,4H2,1-3H3
InchiKey:	PUUCPZKSTXFGOC-UHFFFAOYSA-N
Formula:	C5H12S2
SMILES:	CCSSC(C)C
Mol. weight [g/mol]:	136.28
CAS:	53966-36-2

Physical Properties

Property code	Value	Unit	Source
gf	55.02	kJ/mol	Joback Method
hf	-68.07	kJ/mol	Joback Method
hfus	13.44	kJ/mol	Joback Method
hvap	39.97	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.796		Crippen Method
mcvol	114.010	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
rinpol	985.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	984.00		NIST Webbook
ripol	1319.00		NIST Webbook
ripol	1319.00		NIST Webbook
tb	438.00 ± 1.50	K	NIST Webbook
tc	671.44	K	Joback Method
tf	199.91	K	Joback Method
vc	0.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.94	J/mol×K	450.92	Joback Method
cpg	225.27	J/mol×K	487.67	Joback Method
cpg	236.10	J/mol×K	524.43	Joback Method
cpg	246.44	J/mol×K	561.18	Joback Method
cpg	256.29	J/mol×K	597.94	Joback Method
cpg	265.64	J/mol×K	634.69	Joback Method
cpg	274.48	J/mol×K	671.44	Joback Method
hvapt	42.50	kJ/mol	397.50	NIST Webbook
hvapt	42.90	kJ/mol	395.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45211e+01
Coeff. B	-3.76979e+03
Coeff. C	-6.30930e+01
Temperature range (K), min.	327.95
Temperature range (K), max.	472.42

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C53966362&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/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
hvapt:	Enthalpy of vaporization at a given temperature
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