Disulfide, bis(3-methylbutyl)

Other names:	2,9-Dimethyl-5,6-dithiadecane
	5,6-Dithia-2,9-dimethyldecane
	Bis(3-methyl-1-butyl) disulfide
	Bis(3-methylbutyl) disulfide
	Diisoamyl disulfide
	Diisopentyl disulfide
	Diisopentyl disulphide
	Isoamyl disulfide
	Isopentyl disulfide
Inchi:	InChI=1S/C10H22S2/c1-9(2)5-7-11-12-8-6-10(3)4/h9-10H,5-8H2,1-4H3
InchiKey:	MPYGLNNTOXLWOB-UHFFFAOYSA-N
Formula:	C10H22S2
SMILES:	CC(C)CCSSCCC(C)C
Mol. weight [g/mol]:	206.41
CAS:	2051-04-9

Physical Properties

Property code	Value	Unit	Source
gf	94.68	kJ/mol	Joback Method
hf	-176.55	kJ/mol	Joback Method
hfus	22.87	kJ/mol	Joback Method
hvap	50.71	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	4.460		Crippen Method
mcvol	184.460	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
rinpol	1409.00		NIST Webbook
rinpol	1409.00		NIST Webbook
ripol	1669.00		NIST Webbook
tb	523.20	K	NIST Webbook
tc	773.35	K	Joback Method
tf	241.26	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.71	J/mol×K	564.88	Joback Method
cpg	452.65	J/mol×K	599.63	Joback Method
cpg	468.73	J/mol×K	634.37	Joback Method
cpg	483.97	J/mol×K	669.12	Joback Method
cpg	498.38	J/mol×K	703.86	Joback Method
cpg	511.98	J/mol×K	738.61	Joback Method
cpg	524.77	J/mol×K	773.35	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46855e+01
Coeff. B	-4.40385e+03
Coeff. C	-8.57520e+01
Temperature range (K), min.	391.62
Temperature range (K), max.	555.55

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=C2051049&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