METHYL ISOPROPYL DISULPHIDE

Other names:	Disulfide, methyl 1-methylethyl
	Methyl i-propyl disulfide
	Methyl isopropyl disulfide
	2-Methyl-3,4-dithiapentane
	Isopropyl methyl disulfide
	Disulfide, isopropyl methyl
	isopropyl methyl disulphide
Inchi:	InChI=1S/C4H10S2/c1-4(2)6-5-3/h4H,1-3H3
InchiKey:	MRCFHOIQEFOJEC-UHFFFAOYSA-N
Formula:	C4H10S2
SMILES:	CSSC(C)C
Mol. weight [g/mol]:	122.26

Physical Properties

Property code	Value	Unit	Source
af	0.2483		Cheméo Relay (1.0)
hf	-79.10	kJ/mol	NIST Webbook
hfus	10.85	kJ/mol	Joback Method
hvap	39.55	kJ/mol	Cheméo Relay (1.0)
ie	8.48	eV	Cheméo Relay (1.0)
logp	2.406		Crippen Method
mcvol	99.920	ml/mol	McGowan Method
pc	4109.14	kPa	Joback Method
rinpol	899.00		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	906.00		NIST Webbook
ripol	1192.00		NIST Webbook
ripol	1221.00		NIST Webbook
ripol	1192.00		NIST Webbook
ripol	1192.00		NIST Webbook
ripol	1192.00		NIST Webbook
tb	410.40	K	Cheméo Relay (1.0)
tc	618.36	K	Cheméo Relay (1.0)
tf	181.78	K	Cheméo Relay (1.0)
vc	0.351	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	175.92	J/mol×K	428.04	Joback Method
cpg	185.72	J/mol×K	465.32	Joback Method
cpg	195.12	J/mol×K	502.59	Joback Method
cpg	204.11	J/mol×K	539.87	Joback Method
cpg	212.69	J/mol×K	577.15	Joback Method
cpg	220.86	J/mol×K	614.42	Joback Method
cpg	228.60	J/mol×K	651.70	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C40136650&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical 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