

ISOPROPYL ISOBUTYL DISULPHIDE

Other names:	2,6-Dimethyl-3,4-dithiaheptane
Inchi:	InChI=1S/C7H16S2/c1-6(2)5-8-9-7(3)4/h6-7H,5H2,1-4H3
InchiKey:	IYFXKQOEFVPRQY-UHFFFAOYSA-N
Formula:	C7H16S2
SMILES:	CC(C)CSSC(C)C
Mol. weight [g/mol]:	164.34

Physical Properties

Property code	Value	Unit	Source
hf	-147.33	kJ/mol	Cheméo Relay (1.0)
hfus	15.10	kJ/mol	Joback Method
hvap	51.91	kJ/mol	Cheméo Relay (1.0)
ie	8.26	eV	Cheméo Relay (1.0)
logp	3.432		Crippen Method
mcvol	142.190	ml/mol	McGowan Method
rmpol	1118.00		NIST Webbook
rmpol	1118.00		NIST Webbook
tb	460.47	K	Cheméo Relay (1.0)
tf	195.15	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.83	J/mol×K	496.24	Joback Method
cpg	311.09	J/mol×K	532.73	Joback Method
cpg	324.67	J/mol×K	569.21	Joback Method
cpg	337.56	J/mol×K	605.70	Joback Method
cpg	349.78	J/mol×K	642.19	Joback Method
cpg	361.33	J/mol×K	678.67	Joback Method
cpg	372.21	J/mol×K	715.16	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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=C67421823&Units=SI

Legend

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/15-364-1/ISOPROPYL-ISOBUTYL-DISULPHIDE.pdf>

Generated by Cheméo on 2026-07-21 20:55:07.420819173 +0000 UTC m=+178403.262704548.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.