

Disulfide, 1-methylethyl propyl

Other names: 1-(Isopropyldisulfanyl)propane; 2-Methyl-3,4-dithiaheptane; Disulfide, isopropyl propyl; Isopropyl propyl disulfide; Propyl isopropyl disulfide; isopropyl propyl disulphide.

InChI: InChI=1S/C6H14S2/c1-4-5-7-8-6(2)3/h6H,4-5H2,1-3H3

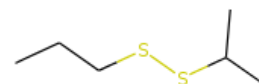
InChI Key: YCBVTHJPQCNICU-UHFFFAOYSA-N

Formula: C6H14S2

SMILES: CCCSSC(C)C

Molecular Weight: 150.30

CAS: 33672-51-4



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	63.44	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-88.71	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	16.03	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	42.20	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.19		Crippen Method
P_c	3257.86	kPa	Joback Method
T_{boil}	457.00 ± 1.70	K	NIST Webbook
T_c	691.06	K	Joback Method
T_{fus}	211.18	K	Joback Method
V_c	0.47	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	254.21	J/mol×K	473.8	Joback Method
$\Delta_{\text{vap}} H$	45.40	kJ/mol	408.0	NIST Webbook

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C6H14S2/c1-4-5-7-8-6\(2\)3/h6H,4-5H2,1-3H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C6H14S2/c1-4-5-7-8-6(2)3/h6H,4-5H2,1-3H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$C_{p, \text{gas}}$: Ideal gas heat capacity (J/mol×K).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{\text{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{\text{fus}} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{\text{vap}} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$\Delta_{\text{vap}} H$: Enthalpy of vaporization at a given temperature (kJ/mol).

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

P_c : Critical Pressure (kPa).

T_{boil} : Normal Boiling Point Temperature (K).

T_c : Critical Temperature (K).

T_{fus} : Normal melting (fusion) point (K).

V_c : Critical Volume (m³/kg-mol).

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