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

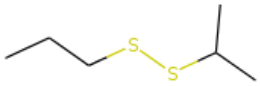
InChI Key: YCBVTHJPQCNICU-UHFFFAOYSA-N

Formula: C6H14S2

SMILES: CCCSSC(C)C

Molecular Weight: 150.30

CAS: 33672-51-4



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	63.44	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-88.71	kJ/mol	Joback Method
$\Delta_{fus} H°$	16.03	kJ/mol	Joback Method
$\Delta_{vap} H°$	42.20	kJ/mol	Joback Method
$logP_{oct/wat}$	3.186		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	0.473	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	254.21	J/mol×K	473.8	Joback Method
$\Delta_{vap} H$	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
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
$\mathbf{\Delta_f G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\mathbf{\Delta_f H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\mathbf{\Delta_{fus} H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\mathbf{\Delta_{vap} H}$: Enthalpy of vaporization at a given temperature (kJ/mol).
$\mathbf{\mathit{log} P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).

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