

Sulfide, isobutyl isopropyl

Other names:	Propane, 2-methyl-1-[(1-methylethyl)thio]- 1-(Isopropylsulfanyl)-2-methylpropane 2,5-Dimethyl-3-thiahexane Isopropyl isobutyl sulfide
Inchi:	InChI=1S/C7H16S/c1-6(2)5-8-7(3)4/h6-7H,5H2,1-4H3
InchiKey:	NAPBMSIZYSDRMH-UHFFFAOYSA-N
Formula:	C7H16S
SMILES:	CC(C)CSC(C)C
Mol. weight [g/mol]:	132.27
CAS:	10359-65-6

Physical Properties

Property code	Value	Unit	Source
gf	36.30	kJ/mol	Joback Method
hf	-156.50	kJ/mol	Joback Method
hfus	10.97	kJ/mol	Joback Method
hvap	37.22	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.784		Crippen Method
mcvol	125.840	ml/mol	McGowan Method
pc	2899.85	kPa	Joback Method
rinpol	895.00		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	895.00		NIST Webbook
rinpol	895.00		NIST Webbook
tb	427.46	K	Joback Method
tc	623.67	K	Joback Method
tf	173.05	K	Joback Method
vc	0.469	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.67	J/molxK	427.46	Joback Method

cpg	259.20	J/mol×K	460.16	Joback Method
cpg	272.18	J/mol×K	492.86	Joback Method
cpg	284.59	J/mol×K	525.56	Joback Method
cpg	296.47	J/mol×K	558.26	Joback Method
cpg	307.81	J/mol×K	590.96	Joback Method
cpg	318.62	J/mol×K	623.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10359656&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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