

Propane, 1-[(1-methylethyl)thio]-

Other names:	Sulfide, isopropyl propyl n-Propyl isopropyl sulfide Isopropylpropyl sulfide Propyl isopropyl sulfide 1-[(1-methylethyl)thio]propane
Inchi:	InChI=1S/C6H14S/c1-4-5-7-6(2)3/h6H,4-5H2,1-3H3
InchiKey:	BDFDQOJJDDORSR-UHFFFAOYSA-N
Formula:	C6H14S
SMILES:	CCCSC(C)C
Mol. weight [g/mol]:	118.24
CAS:	5008-73-1

Physical Properties

Property code	Value	Unit	Source
gf	30.32	kJ/mol	Joback Method
hf	-130.58	kJ/mol	Joback Method
hfus	11.90	kJ/mol	Joback Method
hvap	41.80	kJ/mol	NIST Webbook
log10ws	-2.33		Crippen Method
logp	2.538		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
rinpola	839.00		NIST Webbook
rinpola	839.00		NIST Webbook
rinpola	839.00		NIST Webbook
rinpola	839.00		NIST Webbook
tb	405.30 ± 0.40	K	NIST Webbook
tc	598.38	K	Joback Method
tf	176.78	K	Joback Method
vc	0.419	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	251.08	J/mol×K	533.93	Joback Method
cpg	261.10	J/mol×K	566.16	Joback Method
cpg	206.46	J/mol×K	405.02	Joback Method
cpg	218.30	J/mol×K	437.25	Joback Method
cpg	229.68	J/mol×K	469.47	Joback Method
cpg	240.61	J/mol×K	501.70	Joback Method
cpg	270.69	J/mol×K	598.38	Joback Method
hvapt	41.10	kJ/mol	367.50	NIST Webbook
hvapt	39.00	kJ/mol	379.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5008731&Units=SI

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
hvac:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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