

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

Other names:	Sulfide, butyl isopropyl Butyl isopropyl sulfide
Inchi:	InChI=1S/C7H16S/c1-4-5-6-8-7(2)3/h7H,4-6H2,1-3H3
InchiKey:	QIAZGMDOMXLGBB-UHFFFAOYSA-N
Formula:	C7H16S
SMILES:	CCCCSC(C)C
Mol. weight [g/mol]:	132.27
CAS:	7309-43-5

Physical Properties

Property code	Value	Unit	Source
gf	38.74	kJ/mol	Joback Method
hf	-151.22	kJ/mol	Joback Method
hfus	14.49	kJ/mol	Joback Method
hvap	37.61	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.928		Crippen Method
mcvol	125.840	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
rinpol	936.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	936.00		NIST Webbook
tb	417.75 ± 0.30	K	NIST Webbook
tc	619.57	K	Joback Method
tf	188.05	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.63	J/mol×K	427.90	Joback Method
cpg	258.76	J/mol×K	459.85	Joback Method
cpg	271.36	J/mol×K	491.79	Joback Method

cpg	283.45	J/mol×K	523.74	Joback Method
cpg	295.02	J/mol×K	555.68	Joback Method
cpg	306.08	J/mol×K	587.63	Joback Method
cpg	316.66	J/mol×K	619.57	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7309435&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
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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