Sulfide, sec-butyl isopropyl

Other names:	Butane, 2-[(1-methylethyl)thio]-
	Sec-butyl isopropyl sulfide
	2,4-dimethyl-3-thiahexane
	Isopropyl 2-butyl sulfide
	Isopropyl (1-methylpropyl) sulfide
	Sulfide, 1-methylethyl 1-methylpropyl
Inchi:	InChI=1S/C7H16S/c1-5-7(4)8-6(2)3/h6-7H,5H2,1-4H3
InchiKey:	QFJOWMMNNIEXPT-UHFFFAOYSA-N
Formula:	C7H16S
SMILES:	CCC(C)SC(C)C
Mol. weight [g/mol]:	132.27
CAS:	22438-36-4

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	-2.86		Crippen Method
logp	2.926		Crippen Method
mcvol	125.840	ml/mol	McGowan Method
pc	2899.85	kPa	Joback Method
rinpol	887.00		NIST Webbook
rinpol	897.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	886.00		NIST Webbook
rinpol	890.00		NIST Webbook
rinpol	887.00		NIST Webbook
tb	427.46	K	Joback Method
tc	623.67	K	Joback Method
tf	173.05	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.67	J/mol×K	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

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=C22438364&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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