

Pentane, 1-[(3-methylbutyl)thio]-

Other names:	Sulfide, isopentyl pentyl 1-(Isopentylsulfanyl)pentane 2-Methyl-5-thiadecane Pentyl isopentyl sulfide
Inchi:	InChI=1S/C10H22S/c1-4-5-6-8-11-9-7-10(2)3/h10H,4-9H2,1-3H3
InchiKey:	XUNPTYBWYTYKIS-UHFFFAOYSA-N
Formula:	C10H22S
SMILES:	CCCCCSCCC(C)C
Mol. weight [g/mol]:	174.35
CAS:	7352-01-4

Physical Properties

Property code	Value	Unit	Source
gf	64.00	kJ/mol	Joback Method
hf	-213.14	kJ/mol	Joback Method
hfus	22.26	kJ/mol	Joback Method
hvap	44.28	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.956		Crippen Method
mcvol	168.110	ml/mol	McGowan Method
pc	2157.31	kPa	Joback Method
rinpol	1237.00		NIST Webbook
rinpol	1237.00		NIST Webbook
rinpol	1237.00		NIST Webbook
tb	496.54	K	Joback Method
tc	682.34	K	Joback Method
tf	221.86	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.11	J/mol×K	496.54	Joback Method
cpg	392.28	J/mol×K	527.51	Joback Method

cpg	407.76	J/mol×K	558.47	Joback Method
cpg	422.57	J/mol×K	589.44	Joback Method
cpg	436.72	J/mol×K	620.41	Joback Method
cpg	450.23	J/mol×K	651.37	Joback Method
cpg	463.12	J/mol×K	682.34	Joback Method

Sources

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=C7352014&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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