

Butane, 2-(methylthio)-

Other names:	2-(Methylthio)butane 3-Methyl-2-thiapentane Methyl 2-butyl sulfide Methyl sec-butyl sulfide Sulfide, sec-butyl methyl sec-Butyl methyl sulfide
Inchi:	InChI=1S/C5H12S/c1-4-5(2)6-3/h5H,4H2,1-3H3
InchiKey:	IJRCRFQMYAJPP0-UHFFFAOYSA-N
Formula:	C5H12S
SMILES:	CCC(C)SC
Mol. weight [g/mol]:	104.21
CAS:	10359-64-5

Physical Properties

Property code	Value	Unit	Source
gf	21.90	kJ/mol	Joback Method
hf	-109.94	kJ/mol	Joback Method
hfus	9.31	kJ/mol	Joback Method
hvap	33.15	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	2.148		Crippen Method
mcvol	97.660	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
rinpol	784.00		NIST Webbook
rinpol	790.00		NIST Webbook
rinpol	805.00		NIST Webbook
rinpol	780.00		NIST Webbook
rinpol	796.00		NIST Webbook
rinpol	780.00		NIST Webbook
rinpol	773.00		NIST Webbook
rinpol	780.00		NIST Webbook
tb	382.14	K	Joback Method
tc	576.94	K	Joback Method
tf	165.51	K	Joback Method
vc	0.363	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.65	J/mol×K	382.14	Joback Method
cpg	180.05	J/mol×K	414.61	Joback Method
cpg	190.07	J/mol×K	447.07	Joback Method
cpg	199.69	J/mol×K	479.54	Joback Method
cpg	208.93	J/mol×K	512.01	Joback Method
cpg	217.80	J/mol×K	544.47	Joback Method
cpg	226.28	J/mol×K	576.94	Joback Method
hvapt	38.50	kJ/mol	353.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.43479e+01
Coeff. B	-3.03162e+03
Coeff. C	-6.69910e+01
Temperature range (K), min.	282.61
Temperature range (K), max.	402.48

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=C10359645&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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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