Butane, 3-methyl-1-(methylthio)-

Other names:	(3-Methylbutyl) methyl sulfide
	3-Methyl-1-(methylsulfanyl)butane
	5-Methyl-2-thiahexane
	Methyl isopentyl sulfide
	Sulfide, isopentyl methyl
Inchi:	InChI=1S/C6H14S/c1-6(2)4-5-7-3/h6H,4-5H2,1-3H3
InchiKey:	ABIKQXWLJOURPN-UHFFFAOYSA-N
Formula:	C6H14S
SMILES:	CSCCC(C)C
Mol. weight [g/mol]:	118.24
CAS:	13286-90-3

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	35.38	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	2.396		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
rinpol	862.00		NIST Webbook
rinpol	870.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	864.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	880.00		NIST Webbook
tb	405.02	K	Joback Method
tc	598.38	K	Joback Method
tf	176.78	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	251.08	J/mol×K	533.93	Joback Method
cpg	261.10	J/mol×K	566.16	Joback Method
cpg	270.69	J/mol×K	598.38	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55217e+01
Coeff. B	-3.80046e+03
Coeff. C	-5.54500e+01
Temperature range (K), min.	304.92
Temperature range (K), max.	427.67

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13286903&Units=SI

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

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

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