Butane, 2-methyl-2-(methylthio)-

Other names:	2-Methyl-2-(methylsulfanyl)butane
	3,3-Dimethyl-2-thiapentane
	Methyl tert-pentyl sulfide
	Sulfide, methyl tert-pentyl
Inchi:	InChI=1S/C6H14S/c1-5-6(2,3)7-4/h5H2,1-4H3
InchiKey:	SJOHDSPLOVBXOF-UHFFFAOYSA-N
Formula:	C6H14S
SMILES:	CCC(C)(C)SC
Mol. weight [g/mol]:	118.24
CAS:	13286-92-5

Physical Properties

Property code	Value	Unit	Source
gf	35.60	kJ/mol	Joback Method
hf	-134.05	kJ/mol	Joback Method
hfus	8.01	kJ/mol	Joback Method
hvap	34.47	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.538		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3235.66	kPa	Joback Method
rinpol	847.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	847.00		NIST Webbook
tb	402.23	K	Joback Method
tc	604.13	K	Joback Method
tf	194.20	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.29	J/mol×K	402.23	Joback Method

cpg	221.25	J/mol×K	435.88	Joback Method
cpg	233.54	J/mol×K	469.53	Joback Method
cpg	245.18	J/mol×K	503.18	Joback Method
cpg	256.20	J/mol×K	536.83	Joback Method
cpg	266.61	J/mol×K	570.48	Joback Method
cpg	276.44	J/mol×K	604.13	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.69742e+01
Coeff. B	-4.26602e+03
Coeff. C	-5.87440e+01
Temperature range (K), min.	314.40
Temperature range (K), max.	424.53

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13286925&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