

Propane, 2-methyl-2-(methylthio)-

Other names:	(CH ₃) ₃ CSCH ₃ 2-Methyl-2-(methylthio)-propane 3,3-DIMETHYL-2-THIABUTANE Methyl t-butyl sulfide Methyl tert-butyl sulfide NSC 97331 Sulfide, tert-butyl methyl tert-Butyl methyl sulfide tert-Butyl methyl sulphide
Inchi:	InChI=1S/C5H12S/c1-5(2,3)6-4/h1-4H3
InchiKey:	CJFVCTVYZFTORU-UHFFFAOYSA-N
Formula:	C ₅ H ₁₂ S
SMILES:	CSC(C)(C)C
Mol. weight [g/mol]:	104.21
CAS:	6163-64-0

Physical Properties

Property code	Value	Unit	Source
chl	-4127.20 ± 0.63	kJ/mol	NIST Webbook
gf	27.18	kJ/mol	Joback Method
hf	-121.00 ± 0.75	kJ/mol	NIST Webbook
hfl	-156.90 ± 0.75	kJ/mol	NIST Webbook
hfus	5.42	kJ/mol	Joback Method
hvap	35.80	kJ/mol	NIST Webbook
hvap	35.90	kJ/mol	NIST Webbook
hvap	35.90	kJ/mol	NIST Webbook
hvap	34.20	kJ/mol	NIST Webbook
hvap	35.90	kJ/mol	NIST Webbook
ie	8.38 ± 0.05	eV	NIST Webbook
log10ws	-1.91		Crippen Method
logp	2.148		Crippen Method
mcvol	97.660	ml/mol	McGowan Method
pc	3620.24	kPa	Joback Method
rinpol	724.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	725.00		NIST Webbook

rinpol	724.00		NIST Webbook
rinpol	710.00		NIST Webbook
sl	276.14	J/molxK	NIST Webbook
tb	372.10	K	NIST Webbook
tb	372.05 ± 0.20	K	NIST Webbook
tb	372.20 ± 0.50	K	NIST Webbook
tb	372.10 ± 0.30	K	NIST Webbook
tb	375.00 ± 4.00	K	NIST Webbook
tb	374.70	K	NIST Webbook
tc	569.80	K	NIST Webbook
tf	190.90 ± 0.30	K	NIST Webbook
tf	190.85 ± 0.20	K	NIST Webbook
tt	190.84 ± 0.02	K	NIST Webbook
tt	184.86 ± 0.06	K	NIST Webbook
vc	0.358	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.93	J/molxK	515.08	Joback Method
cpg	231.97	J/molxK	582.94	Joback Method
cpg	223.21	J/molxK	549.01	Joback Method
cpg	171.13	J/molxK	379.35	Joback Method
cpg	182.72	J/molxK	413.28	Joback Method
cpg	193.70	J/molxK	447.21	Joback Method
cpg	204.10	J/molxK	481.15	Joback Method
cpl	199.95	J/molxK	298.15	NIST Webbook
hfust	8.41	kJ/mol	190.80	NIST Webbook
hfust	8.41	kJ/mol	190.84	NIST Webbook
hfust	8.41	kJ/mol	190.80	NIST Webbook
hvapt	35.10	kJ/mol	358.00	NIST Webbook
hvapt	36.50	kJ/mol	336.50	NIST Webbook
hvapt	31.47	kJ/mol	372.10	NIST Webbook
sfust	44.09	J/molxK	190.84	NIST Webbook

Correlations

Information

Value

Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.38760e+01
Coeff. B	-2.99505e+03
Coeff. C	-4.94790e+01
Temperature range (K), min.	269.89
Temperature range (K), max.	399.18

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	7.81918e+01
Coeff. B	-6.79559e+03
Coeff. C	-9.50787e+00
Coeff. D	7.00157e-06
Temperature range (K), min.	306.15
Temperature range (K), max.	410.15

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
KDB:	https://www.therc.org/files/research/kdb/mol/mol1831.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6163640&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.therc.org/research/kdb/hcprop/showprop.php?cmpid=1831

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions

hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpolar:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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