

Benzenemethanethiol

Other names:	(Mercaptomethyl)benzene Benzyl mercaptan Benzylhydrosulfide Benzylthiol Methanethiol, phenyl- NSC 41897 Phenylmethanethiol Phenylmethyl mercaptan Thiobenzyl alcohol USAF ex-1509 toluene-«alpha»-thiol toluene-Â«alphaÂ»-thiol «alpha»-Mercaptotoluene «alpha»-Toluenethiol «alpha»-Toluolthiol «alpha»-Tolyl mercaptan Â«alphaÂ»-Mercaptotoluene Â«alphaÂ»-Toluenethiol Â«alphaÂ»-Toluolthiol Â«alphaÂ»-Tolyl mercaptan
Inchi:	InChI=1S/C7H8S/c8-6-7-4-2-1-3-5-7/h1-5,8H,6H2
InchiKey:	UENWRTRMUIOCKN-UHFFFAOYSA-N
Formula:	C7H8S
SMILES:	SCc1ccccc1
Mol. weight [g/mol]:	124.20
CAS:	100-53-8

Physical Properties

Property code	Value	Unit	Source
chl	-4536.40 ± 1.00	kJ/mol	NIST Webbook
chl	-4544.10 ± 2.00	kJ/mol	NIST Webbook
gf	149.86	kJ/mol	Joback Method
hf	87.70 ± 2.00	kJ/mol	NIST Webbook
hf	93.10 ± 1.10	kJ/mol	NIST Webbook
hfl	36.50 ± 1.10	kJ/mol	NIST Webbook
hfl	43.90 ± 2.10	kJ/mol	NIST Webbook
hfus	11.97	kJ/mol	Joback Method

hvap	43.80	kJ/mol	NIST Webbook
hvap	56.60 ± 0.20	kJ/mol	NIST Webbook
hvap	56.60	kJ/mol	NIST Webbook
hvap	51.00 ± 2.00	kJ/mol	NIST Webbook
hvap	56.60 ± 0.10	kJ/mol	NIST Webbook
ie	8.50	eV	NIST Webbook
ie	8.85	eV	NIST Webbook
log10ws	-2.42		Crippen Method
logp	2.116		Crippen Method
mcvol	102.080	ml/mol	McGowan Method
pc	4474.22	kPa	Joback Method
rinpol	1104.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1067.00		NIST Webbook
rinpol	1067.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1080.00		NIST Webbook
ripol	1615.00		NIST Webbook
ripol	1615.00		NIST Webbook
ripol	1631.00		NIST Webbook
ripol	1618.00		NIST Webbook
ripol	1626.00		NIST Webbook
ripol	1615.00		NIST Webbook
ripol	1631.00		NIST Webbook
tb	468.00	K	NIST Webbook
tb	468.00 ± 3.00	K	NIST Webbook
tb	467.00 ± 3.00	K	NIST Webbook
tb	467.15 ± 2.00	K	NIST Webbook
tb	467.70	K	NIST Webbook
tc	688.15	K	Joback Method
tf	231.53	K	Joback Method
vc	0.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.23	J/mol×K	449.10	Joback Method
cpg	193.19	J/mol×K	488.94	Joback Method
cpg	204.33	J/mol×K	528.78	Joback Method
cpg	214.68	J/mol×K	568.63	Joback Method

cpg	224.29	J/mol×K	608.47	Joback Method
cpg	233.19	J/mol×K	648.31	Joback Method
cpg	241.43	J/mol×K	688.15	Joback Method
hvapt	47.50	kJ/mol	415.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.46319e+01
Coeff. B	-3.96941e+03
Coeff. C	-7.12960e+01
Temperature range (K), min.	348.02
Temperature range (K), max.	497.18

Sources

The Yaws Handbook of Vapor Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<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

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C100538&Units=SI>

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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