Benzene, [(ethylthio)methyl]-

Other names:	Sulfide, benzyl ethyl
	«alpha»-(Ethylthio)toluene
	Benzyl ethyl sulfide
	Ethyl benzyl sulfide
	1-Phenyl-2-thiabutane
Inchi:	InChI=1S/C9H12S/c1-2-10-8-9-6-4-3-5-7-9/h3-7H,2,8H2,1H3
InchiKey:	NTAIOEZEVLVLLW-UHFFFAOYSA-N
Formula:	C9H12S
SMILES:	CCSCc1ccccc1
Mol. weight [g/mol]:	152.26
CAS:	6263-62-3

Physical Properties

Property code	Value	Unit	Source
chl	-5853.20 ± 2.10	kJ/mol	NIST Webbook
gf	170.43	kJ/mol	Joback Method
hf	52.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-5.20 ± 2.20	kJ/mol	NIST Webbook
hfus	17.24	kJ/mol	Joback Method
hvap	57.20	kJ/mol	NIST Webbook
hvap	56.90 ± 2.10	kJ/mol	NIST Webbook
hvap	57.00 ± 2.00	kJ/mol	NIST Webbook
log10ws	-3.07		Crippen Method
logp	2.940		Crippen Method
mcvol	130.260	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
rinpol	1248.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1248.00		NIST Webbook
tb	500.78	K	Joback Method
tc	731.34	K	Joback Method
tf	252.01	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.38	J/mol×K	500.78	Joback Method
cpg	279.81	J/mol×K	539.21	Joback Method
cpg	293.33	J/mol×K	577.63	Joback Method
cpg	305.99	J/mol×K	616.06	Joback Method
cpg	317.80	J/mol×K	654.48	Joback Method
cpg	328.81	J/mol×K	692.91	Joback Method
cpg	339.05	J/mol×K	731.34	Joback Method
hvapt	56.00	kJ/mol	358.00	NIST Webbook
hvapt	54.80	kJ/mol	422.50	NIST Webbook

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6263623&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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