Benzyl methyl disulfide

Other names:	Disulfide, methyl phenylmethyl
	Disulfide, benzyl methyl
	Methyl benzyl disulfide
	benzyl methyl disulphide
Inchi:	InChI=1S/C8H10S2/c1-9-10-7-8-5-3-2-4-6-8/h2-6H,7H2,1H3
InchiKey:	NWYGPVZOBBHKLI-UHFFFAOYSA-N
Formula:	C8H10S2
SMILES:	CSSCc1ccccc1
Mol. weight [g/mol]:	170.29
CAS:	699-10-5

Physical Properties

Property code	Value	Unit	Source
gf	195.13	kJ/mol	Joback Method
hf	111.82	kJ/mol	Joback Method
hfus	18.78	kJ/mol	Joback Method
hvap	49.31	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.198		Crippen Method
mcvol	132.520	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
rinpol	1417.00		NIST Webbook
tb	546.68	K	Joback Method
tc	804.40	K	Joback Method
tf	275.14	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.83	J/mol×K	546.68	Joback Method
cpg	283.35	J/mol×K	589.63	Joback Method
cpg	295.89	J/mol×K	632.59	Joback Method
cpg	307.47	J/mol×K	675.54	Joback Method

cpg	318.12	J/mol×K	718.49	Joback Method
cpg	327.87	J/mol×K	761.45	Joback Method
cpg	336.73	J/mol×K	804.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C699105&Units=SI
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

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