

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]:	170.30

Physical Properties

Property code	Value	Unit	Source
af	0.3388		Cheméo Relay (1.0)
gf	195.13	kJ/mol	Joback Method
hf	110.68	kJ/mol	Cheméo Relay (1.0)
hfus	18.78	kJ/mol	Joback Method
hvap	65.89	kJ/mol	Cheméo Relay (1.0)
ie	8.48	eV	Cheméo Relay (1.0)
log10ws	-2.39		Cheméo Relay (1.0)
logp	3.198		Crippen Method
mcvol	132.520	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
rinpol	1417.00		NIST Webbook
tb	517.24	K	Cheméo Relay (1.0)
tc	751.68	K	Cheméo Relay (1.0)
tf	262.66	K	Cheméo Relay (1.0)
vc	0.458	m3/kmol	Cheméo Relay (1.0)

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C699105&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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