

bis-(1-Propenyl) trisulfide, #2

Inchi:	InChI=1S/C6H10S3/c1-3-5-7-9-8-6-4-2/h3-6H,1-2H3/b5-3+,6-4+
InchiKey:	RWAJLLGQYHTAMT-GGWOSOGESA-N
Formula:	C6H10S3
SMILES:	CC=CSSSC=CC
Mol. weight [g/mol]:	178.34
CAS:	115321-81-8

Physical Properties

Property code	Value	Unit	Source
gf	259.44	kJ/mol	Joback Method
hf	192.88	kJ/mol	Joback Method
hfus	24.09	kJ/mol	Joback Method
hvap	49.32	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.083		Crippen Method
mcvol	135.850	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
rinpol	1327.00		NIST Webbook
rinpol	1348.40		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1348.40		NIST Webbook
tb	551.34	K	Joback Method
tc	808.28	K	Joback Method
tf	250.42	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.86	J/molxK	551.34	Joback Method
cpg	274.32	J/molxK	594.16	Joback Method
cpg	284.97	J/molxK	636.99	Joback Method
cpg	294.84	J/molxK	679.81	Joback Method
cpg	303.97	J/molxK	722.63	Joback Method

cpg	312.40	J/mol×K	765.45	Joback Method
cpg	320.15	J/mol×K	808.28	Joback Method

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C115321818&Units=SI

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
hvac:	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

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