Trisulfide, di-2-propenyl

Other names:	Allyl trisulfide
	Diallyl trisulfide
	diallyl trisulphide
Inchi:	InChI=1S/C6H10S3/c1-3-5-7-9-8-6-4-2/h3-4H,1-2,5-6H2
InchiKey:	UBAXRAHSPKWNCX-UHFFFAOYSA-N
Formula:	C6H10S3
SMILES:	C=CCSSSCC=C
Mol. weight [g/mol]:	178.34
CAS:	2050-87-5

Physical Properties

Property code	Value	Unit	Source
gf	274.68	kJ/mol	Joback Method
hf	209.30	kJ/mol	Joback Method
hfus	21.13	kJ/mol	Joback Method
hvap	48.06	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.388		Crippen Method
mcvol	135.850	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method
rinpol	1275.00		NIST Webbook
rinpol	1266.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1312.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1296.00		NIST Webbook
rinpol	1266.00		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1289.00		NIST Webbook
rinpol	1296.00		NIST Webbook
rinpol	1289.00		NIST Webbook

rinpol	1280.00		NIST Webbook
rinpol	1296.00		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1282.00		NIST Webbook
ripol	1806.00		NIST Webbook
ripol	1822.00		NIST Webbook
ripol	1787.00		NIST Webbook
ripol	1819.00		NIST Webbook
ripol	1805.00		NIST Webbook
ripol	1789.00		NIST Webbook
ripol	1775.00		NIST Webbook
ripol	1784.00		NIST Webbook
ripol	1784.00		NIST Webbook
ripol	1806.00		NIST Webbook
ripol	1806.00		NIST Webbook
tb	536.38	K	Joback Method
tc	781.01	K	Joback Method
tf	257.06	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.89	J/mol×K	536.38	Joback Method
cpg	275.09	J/mol×K	577.15	Joback Method
cpg	285.60	J/mol×K	617.92	Joback Method
cpg	295.43	J/mol×K	658.70	Joback Method
cpg	304.58	J/mol×K	699.47	Joback Method
cpg	313.06	J/mol×K	740.24	Joback Method
cpg	320.87	J/mol×K	781.01	Joback Method

Sources

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=C2050875&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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