

Propyl 2-propenyl trisulfide

Inchi: InChI=1S/C6H12S3/c1-3-5-7-9-8-6-4-2/h3H,1,4-6H2,2H3
InchiKey: IXJMGVJLUBBAQW-UHFFFAOYSA-N
Formula: C6H12S3
SMILES: C=CCSSSCCC
Mol. weight [g/mol]: 180.35
CAS: 33922-73-5

Physical Properties

Property code	Value	Unit	Source
gf	186.84	kJ/mol	Joback Method
hf	83.87	kJ/mol	Joback Method
hfus	22.41	kJ/mol	Joback Method
hvap	48.73	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.612		Crippen Method
mcvol	140.150	ml/mol	McGowan Method
pc	3456.14	kPa	Joback Method
rinpol	1320.60		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1290.00		NIST Webbook
rinpol	1290.00		NIST Webbook
rinpol	1290.00		NIST Webbook
rinpol	1320.60		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1307.00		NIST Webbook
ripol	1797.00		NIST Webbook
ripol	1797.00		NIST Webbook
ripol	1723.00		NIST Webbook
tb	539.70	K	Joback Method
tc	778.74	K	Joback Method
tf	258.82	K	Joback Method
vc	0.514	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.56	J/mol×K	539.70	Joback Method
cpg	294.62	J/mol×K	579.54	Joback Method
cpg	306.00	J/mol×K	619.38	Joback Method
cpg	316.70	J/mol×K	659.22	Joback Method
cpg	326.72	J/mol×K	699.06	Joback Method
cpg	336.06	J/mol×K	738.90	Joback Method
cpg	344.70	J/mol×K	778.74	Joback Method

Sources

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=C33922735&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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