propyl 1-propenyl trisulfide

Inchi: InChI=1S/C6H12S3/c1-3-5-7-9-8-6-4-2/h3,5H,4,6H2,1-2H3/b5-3+
InchiKey: CKVNYTRYOFXVGM-HWKANZROSA-N
Formula: C6H12S3
SMILES: CC=CSSSCCC
Mol. weight [g/mol]: 180.35
CAS: 23838-27-9

Physical Properties

Property code	Value	Unit	Source
gf	179.22	kJ/mol	Joback Method
hf	75.66	kJ/mol	Joback Method
hfus	23.89	kJ/mol	Joback Method
hvap	49.36	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.960		Crippen Method
mcvol	140.150	ml/mol	McGowan Method
pc	3497.14	kPa	Joback Method
rinpol	1339.10		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1322.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1317.00		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1325.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1353.00		NIST Webbook
rinpol	1339.10		NIST Webbook
ripol	1743.00		NIST Webbook
ripol	1765.00		NIST Webbook
ripol	1770.00		NIST Webbook
ripol	1781.00		NIST Webbook
ripol	1770.00		NIST Webbook
ripol	1781.00		NIST Webbook
tb	547.18	K	Joback Method

tc	792.12	K	Joback Method
tf	255.50	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.26	J/mol×K	547.18	Joback Method
cpg	294.48	J/mol×K	588.00	Joback Method
cpg	305.95	J/mol×K	628.83	Joback Method
cpg	316.70	J/mol×K	669.65	Joback Method
cpg	326.73	J/mol×K	710.47	Joback Method
cpg	336.04	J/mol×K	751.29	Joback Method
cpg	344.66	J/mol×K	792.12	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C23838279&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

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