propyl cis-1-propenyl pentasulfide

Inchi: InChI=1S/C6H12S5/c1-3-5-7-9-11-10-8-6-4-2/h3,5H,4,6H2,1-2H3/b5-3-
InchiKey: FIABOFOWKCHXJG-HYXAFXHYSA-N
Formula: C6H12S5
SMILES: CC=CSSSSSCCC
Mol. weight [g/mol]: 244.48

Physical Properties

Property code	Value	Unit	Source
gf	245.46	kJ/mol	Joback Method
hf	159.40	kJ/mol	Joback Method
hfus	32.15	kJ/mol	Joback Method
hvap	62.99	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	5.256		Crippen Method
mcvol	172.850	ml/mol	McGowan Method
pc	3642.13	kPa	Joback Method
rinpol	1822.00		NIST Webbook
rinpol	1822.00		NIST Webbook
tb	684.74	K	Joback Method
tc	968.36	K	Joback Method
tf	324.30	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.98	J/mol×K	684.74	Joback Method
cpg	384.15	J/mol×K	732.01	Joback Method
cpg	395.19	J/mol×K	779.28	Joback Method
cpg	405.08	J/mol×K	826.55	Joback Method
cpg	413.80	J/mol×K	873.82	Joback Method
cpg	421.34	J/mol×K	921.09	Joback Method
cpg	427.68	J/mol×K	968.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R237951&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume