Furfuryl 2-propenyl sulfide

Inchi: InChI=1S/C9H12S/c1-2-7-10-8-9-5-3-4-6-9/h2-5H,1,6-8H2
InchiKey: CVKRNHDVHYNFHS-UHFFFAOYSA-N
Formula: C9H12S
SMILES: C=CCSCC1=CC=CC1
Mol. weight [g/mol]: 152.26

Physical Properties

Property code	Value	Unit	Source
gf	240.41	kJ/mol	Joback Method
hf	123.12	kJ/mol	Joback Method
hfus	16.84	kJ/mol	Joback Method
hvap	43.59	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.792		Crippen Method
mcvol	130.260	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
rinpol	1144.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1146.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1137.00		NIST Webbook
tb	494.03	K	Joback Method
tc	718.67	K	Joback Method
tf	253.01	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.80	J/mol×K	494.03	Joback Method
cpg	278.85	J/mol×K	531.47	Joback Method
cpg	292.01	J/mol×K	568.91	Joback Method

cpg	304.31	J/mol×K	606.35	Joback Method
cpg	315.80	J/mol×K	643.79	Joback Method
cpg	326.51	J/mol×K	681.23	Joback Method
cpg	336.50	J/mol×K	718.67	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R43887&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
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