Furfuryl 2-methyl-2-propenyl sulfide

Inchi: InChI=1S/C10H14S/c1-9(2)7-11-8-10-5-3-4-6-10/h3-5H,1,6-8H2,2H3
InchiKey: WPTWMMCUSDCDCL-UHFFFAOYSA-N
Formula: C10H14S
SMILES: C=C(C)CSCC1=CC=CC1
Mol. weight [g/mol]: 166.28

Physical Properties

Property code	Value	Unit	Source
gf	240.28	kJ/mol	Joback Method
hf	92.69	kJ/mol	Joback Method
hfus	18.12	kJ/mol	Joback Method
hvap	45.89	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	3.182		Crippen Method
mcvol	144.350	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
rinpol	1226.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1218.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1216.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1223.00		NIST Webbook
tb	516.79	K	Joback Method
tc	741.94	K	Joback Method
tf	250.32	K	Joback Method
vc	0.545	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.66	J/mol×K	516.79	Joback Method
cpg	323.91	J/mol×K	554.32	Joback Method

cpg	338.20	J/mol×K	591.84	Joback Method
cpg	351.56	J/mol×K	629.37	Joback Method
cpg	364.04	J/mol×K	666.89	Joback Method
cpg	375.70	J/mol×K	704.42	Joback Method
cpg	386.58	J/mol×K	741.94	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=R43873&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume