Furfuryl propyl sulfide

Inchi: InChI=1S/C9H14S/c1-2-7-10-8-9-5-3-4-6-9/h3-5H,2,6-8H2,1H3
InchiKey: VJJASIQQMJJVSP-UHFFFAOYSA-N
Formula: C9H14S
SMILES: CCCSCC1=CC=CC1
Mol. weight [g/mol]: 154.27

Physical Properties

Property code	Value	Unit	Source
gf	152.57	kJ/mol	Joback Method
hf	-2.31	kJ/mol	Joback Method
hfus	18.11	kJ/mol	Joback Method
hvap	44.26	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	3.016		Crippen Method
mcvol	134.560	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
rinpol	1149.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1156.00		NIST Webbook
tb	497.35	K	Joback Method
tc	716.98	K	Joback Method
tf	254.77	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.56	J/mol×K	497.35	Joback Method
cpg	297.32	J/mol×K	533.95	Joback Method
cpg	311.21	J/mol×K	570.56	Joback Method
cpg	324.26	J/mol×K	607.16	Joback Method

cpg	336.52	J/mol×K	643.77	Joback Method
cpg	348.01	J/mol×K	680.37	Joback Method
cpg	358.77	J/mol×K	716.98	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=R43908&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