Isobutyl furfuryl sulfide

Inchi: InChI=1S/C11H18S/c1-10(2)7-8-12-9-11-5-3-4-6-11/h3-5,10H,6-9H2,1-2H3
InchiKey: NXPWMLYKOOSTEU-UHFFFAOYSA-N
Formula: C11H18S
SMILES: CC(C)CCSCC1=CC=CC1
Mol. weight [g/mol]: 182.33

Physical Properties

Property code	Value	Unit	Source
gf	166.97	kJ/mol	Joback Method
hf	-48.87	kJ/mol	Joback Method
hfus	19.77	kJ/mol	Joback Method
hvap	48.32	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.652		Crippen Method
mcvol	162.740	ml/mol	McGowan Method
pc	2553.34	kPa	Joback Method
rinpol	1202.00		NIST Webbook
rinpol	1201.00		NIST Webbook
rinpol	1209.00		NIST Webbook
rinpol	1212.00		NIST Webbook
rinpol	1214.00		NIST Webbook
rinpol	1201.00		NIST Webbook
rinpol	1207.00		NIST Webbook
tb	542.67	K	Joback Method
tc	759.88	K	Joback Method
tf	262.31	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.26	J/mol×K	542.67	Joback Method
cpg	391.14	J/mol×K	578.87	Joback Method
cpg	407.03	J/mol×K	615.07	Joback Method

cpg	421.96	J/mol×K	651.28	Joback Method
cpg	435.98	J/mol×K	687.48	Joback Method
cpg	449.12	J/mol×K	723.68	Joback Method
cpg	461.43	J/mol×K	759.88	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=R43912&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