Furfuryl pentyl sulfide

Inchi: InChI=1S/C11H18S/c1-2-3-6-9-12-10-11-7-4-5-8-11/h4-5,7H,2-3,6,8-10H2,1H3
InchiKey: FJJCNPGLUDLZMD-UHFFFAOYSA-N
Formula: C11H18S
SMILES: CCCCCSCC1=CC=CC1
Mol. weight [g/mol]: 182.33

Physical Properties

Property code	Value	Unit	Source
gf	169.41	kJ/mol	Joback Method
hf	-43.59	kJ/mol	Joback Method
hfus	23.29	kJ/mol	Joback Method
hvap	48.71	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.796		Crippen Method
mcvol	162.740	ml/mol	McGowan Method
pc	2532.82	kPa	Joback Method
rinpol	1354.00		NIST Webbook
rinpol	1352.00		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1349.00		NIST Webbook
rinpol	1354.00		NIST Webbook
rinpol	1346.00		NIST Webbook
tb	543.11	K	Joback Method
tc	755.61	K	Joback Method
tf	277.31	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.96	J/mol×K	543.11	Joback Method
cpg	390.41	J/mol×K	578.53	Joback Method
cpg	405.92	J/mol×K	613.94	Joback Method
cpg	420.52	J/mol×K	649.36	Joback Method

cpg	434.25	J/mol×K	684.77	Joback Method
cpg	447.16	J/mol×K	720.19	Joback Method
cpg	459.27	J/mol×K	755.61	Joback Method

Sources

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=R43891&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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