Bis(2-methyl-4,5-dihydro-3-furyl) Disulfide

Inchi: InChI=1S/C10H14O2S2/c1-7-9(3-5-11-7)13-14-10-4-6-12-8(10)2/h3-6H2,1-2H3
InchiKey: KMPMFKJGGUSVMW-UHFFFAOYSA-N
Formula: C10H14O2S2
SMILES: CC1=C(SSC2=C(C)OCC2)CCO1
Mol. weight [g/mol]: 230.35

Physical Properties

Property code	Value	Unit	Source
gf	37.24	kJ/mol	Joback Method
hf	-198.67	kJ/mol	Joback Method
hfus	32.49	kJ/mol	Joback Method
hvap	64.87	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.671		Crippen Method
mcvol	165.880	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
rinpol	1676.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1676.00		NIST Webbook
rinpol	1676.00		NIST Webbook
tb	677.80	K	Joback Method
tc	943.49	K	Joback Method
tf	406.28	K	Joback Method
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.99	J/mol×K	677.80	Joback Method
cpg	437.14	J/mol×K	722.08	Joback Method
cpg	451.07	J/mol×K	766.36	Joback Method
cpg	463.82	J/mol×K	810.64	Joback Method
cpg	475.42	J/mol×K	854.92	Joback Method
cpg	485.93	J/mol×K	899.21	Joback Method

cpg	495.38	J/mol×K	943.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U365974&Units=SI
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

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