bis-(2-Methyldihydrofuryl-3-) disulfide

Inchi: InChI=1S/C10H14O2S2/c1-7-9(3-5-11-7)13-14-10-4-6-12-8(10)2/h3-10H,1-2H3
InchiKey: PGDKPVCNQBBCCW-UHFFFAOYSA-N
Formula: C10H14O2S2
SMILES: CC1OC=CC1SSC1C=COC1C
Mol. weight [g/mol]: 230.35

Physical Properties

Property code	Value	Unit	Source
gf	44.92	kJ/mol	Joback Method
hf	-234.15	kJ/mol	Joback Method
hfus	38.33	kJ/mol	Joback Method
hvap	60.99	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	2.970		Crippen Method
mcvol	165.880	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
rinpol	1538.00		NIST Webbook
rinpol	1538.00		NIST Webbook
tb	639.20	K	Joback Method
tc	902.36	K	Joback Method
tf	339.24	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.21	J/mol×K	639.20	Joback Method
cpg	454.64	J/mol×K	683.06	Joback Method
cpg	471.56	J/mol×K	726.92	Joback Method
cpg	486.99	J/mol×K	770.78	Joback Method
cpg	500.97	J/mol×K	814.64	Joback Method
cpg	513.53	J/mol×K	858.50	Joback Method
cpg	524.70	J/mol×K	902.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R125927&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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