1,5-Dithiaspiro[5.7]tridecan-7-ol

Inchi: InChI=1S/C11H20OS2/c12-10-6-3-1-2-4-7-11(10)13-8-5-9-14-11/h10,12H,1-9H2
InchiKey: JVWYOEKYHIUDPT-UHFFFAOYSA-N
Formula: C11H20OS2
SMILES: OC1CCCCCCC12SCCCS2
Mol. weight [g/mol]: 232.41
CAS: 70068-14-3

Physical Properties

Property code	Value	Unit	Source
gf	15.95	kJ/mol	Joback Method
hf	-214.36	kJ/mol	Joback Method
hfus	10.92	kJ/mol	Joback Method
hvap	68.26	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.268		Crippen Method
mcvol	182.700	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
rinpol	1961.00		NIST Webbook
rinpol	1961.00		NIST Webbook
tb	682.53	K	Joback Method
tc	937.69	K	Joback Method
tf	476.59	K	Joback Method
vc	0.619	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.46	J/mol×K	682.53	Joback Method
cpg	530.33	J/mol×K	725.06	Joback Method
cpg	548.95	J/mol×K	767.58	Joback Method
cpg	566.52	J/mol×K	810.11	Joback Method
cpg	583.24	J/mol×K	852.64	Joback Method
cpg	599.30	J/mol×K	895.16	Joback Method
cpg	614.93	J/mol×K	937.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C70068143&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