1,14-Dichloro-3,9-dithia-6,12-dioxatetradecane

Inchi: InChI=1S/C10H20Cl2O2S2/c11-1-3-13-4-9-16-10-6-14-5-8-15-7-2-12/h1-10H2
InchiKey: CCXAYKVGTLHLRL-UHFFFAOYSA-N
Formula: C10H20Cl2O2S2
SMILES: ClCCOCCSCCOCCSCCCl
Mol. weight [g/mol]: 307.30

Physical Properties

Property code	Value	Unit	Source
gf	-134.30	kJ/mol	Joback Method
hf	-461.91	kJ/mol	Joback Method
hfus	40.69	kJ/mol	Joback Method
hvap	65.08	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.964		Crippen Method
mcvol	220.680	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	2200.00		NIST Webbook
rinpol	2280.40		NIST Webbook
rinpol	2200.00		NIST Webbook
rinpol	2280.40		NIST Webbook
rinpol	2200.00		NIST Webbook
tb	685.46	K	Joback Method
tc	889.59	K	Joback Method
tf	375.56	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.50	J/mol×K	685.46	Joback Method
cpg	558.40	J/mol×K	719.48	Joback Method
cpg	571.51	J/mol×K	753.50	Joback Method
cpg	583.82	J/mol×K	787.52	Joback Method
cpg	595.32	J/mol×K	821.54	Joback Method

cpg	605.99	J/mol×K	855.56	Joback Method
cpg	615.84	J/mol×K	889.59	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=R41409&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