3,9,12-Trithia-6-oxa-14-chloro-1-tetradecene

Inchi: InChI=1S/C10H19ClOS3/c1-2-13-7-4-12-5-8-15-10-9-14-6-3-11/h2H,1,3-10H2
InchiKey: OCBZLAXMLHXLDP-UHFFFAOYSA-N
Formula: C10H19ClOS3
SMILES: C=CSCCOCCSCCSCCCl
Mol. weight [g/mol]: 286.90

Physical Properties

Property code	Value	Unit	Source
gf	103.59	kJ/mol	Joback Method
hf	-146.65	kJ/mol	Joback Method
hfus	38.15	kJ/mol	Joback Method
hvap	64.43	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.585		Crippen Method
mcvol	214.620	ml/mol	McGowan Method
pc	2185.64	kPa	Joback Method
rinpol	2161.00		NIST Webbook
rinpol	2161.00		NIST Webbook
rinpol	2161.00		NIST Webbook
tb	691.07	K	Joback Method
tc	912.64	K	Joback Method
tf	356.05	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.08	J/mol×K	691.07	Joback Method
cpg	537.28	J/mol×K	728.00	Joback Method
cpg	550.55	J/mol×K	764.93	Joback Method
cpg	562.90	J/mol×K	801.85	Joback Method
cpg	574.31	J/mol×K	838.78	Joback Method
cpg	584.80	J/mol×K	875.71	Joback Method
cpg	594.36	J/mol×K	912.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R41534&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