Undecane, 3,4-bis-(methylthio), erythro

Inchi: InChI=1S/C13H28S2/c1-5-7-8-9-10-11-13(15-4)12(6-2)14-3/h12-13H,5-11H2,1-4H3/t12-,
InchiKey: YRIYGKXBXUSKCI-OLZOCXBDSA-N
Formula: C13H28S2
SMILES: CCCCCCCC(SC)C(CC)SC
Mol. weight [g/mol]: 248.49

Physical Properties

Property code	Value	Unit	Source
gf	119.94	kJ/mol	Joback Method
hf	-238.47	kJ/mol	Joback Method
hfus	30.64	kJ/mol	Joback Method
hvap	57.39	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	5.220		Crippen Method
mcvol	226.730	ml/mol	McGowan Method
pc	1713.19	kPa	Joback Method
rinpol	1745.00		NIST Webbook
rinpol	1745.00		NIST Webbook
tb	633.52	K	Joback Method
tc	832.98	K	Joback Method
tf	275.07	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.75	J/mol×K	633.52	Joback Method
cpg	608.29	J/mol×K	666.76	Joback Method
cpg	625.87	J/mol×K	700.01	Joback Method
cpg	642.51	J/mol×K	733.25	Joback Method
cpg	658.23	J/mol×K	766.50	Joback Method
cpg	673.04	J/mol×K	799.74	Joback Method
cpg	686.98	J/mol×K	832.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R121841&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