Nonadecane, 1,2-bis(methylthio)

Inchi: InChI=1S/C21H44S2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-21(23-3)20-22-2/h2
InchiKey: WMVUSGRBCWIAIO-UHFFFAOYSA-N
Formula: C21H44S2
SMILES: CCCCCCCCCCCCCCCCCC(CSC)SC
Mol. weight [g/mol]: 360.70

Physical Properties

Property code	Value	Unit	Source
gf	189.74	kJ/mol	Joback Method
hf	-398.31	kJ/mol	Joback Method
hfus	54.88	kJ/mol	Joback Method
hvap	75.59	kJ/mol	Joback Method
log10ws	-8.49		Crippen Method
logp	8.342		Crippen Method
mcvol	339.450	ml/mol	McGowan Method
pc	981.46	kPa	Joback Method
rinpol	2687.00		NIST Webbook
rinpol	2687.00		NIST Webbook
tb	817.00	K	Joback Method
tc	1007.88	K	Joback Method
tf	380.23	K	Joback Method
vc	1.313	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1054.71	J/mol×K	817.00	Joback Method
cpg	1075.06	J/mol×K	848.81	Joback Method
cpg	1094.25	J/mol×K	880.63	Joback Method
cpg	1112.30	J/mol×K	912.44	Joback Method
cpg	1129.27	J/mol×K	944.25	Joback Method
cpg	1145.17	J/mol×K	976.07	Joback Method
cpg	1160.05	J/mol×K	1007.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R59303&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