Eicosane, 1,2-bis(methylthio)

Inchi: InChI=1S/C22H46S2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-22(24-3)21-23-2
InchiKey: JBUWPPATFRBVHZ-UHFFFAOYSA-N
Formula: C22H46S2
SMILES: CCCCCCCCCCCCCCCCCCC(CSC)SC
Mol. weight [g/mol]: 374.73

Physical Properties

Property code	Value	Unit	Source
gf	198.16	kJ/mol	Joback Method
hf	-418.95	kJ/mol	Joback Method
hfus	57.47	kJ/mol	Joback Method
hvap	77.81	kJ/mol	Joback Method
log10ws	-8.91		Crippen Method
logp	8.733		Crippen Method
mcvol	353.540	ml/mol	McGowan Method
pc	924.99	kPa	Joback Method
rinpol	2797.00		NIST Webbook
rinpol	2797.00		NIST Webbook
tb	839.88	K	Joback Method
tc	1032.77	K	Joback Method
tf	391.50	K	Joback Method
vc	1.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1117.02	J/mol×K	839.88	Joback Method
cpg	1137.63	J/mol×K	872.03	Joback Method
cpg	1157.03	J/mol×K	904.18	Joback Method
cpg	1175.26	J/mol×K	936.33	Joback Method
cpg	1192.35	J/mol×K	968.47	Joback Method
cpg	1208.35	J/mol×K	1000.62	Joback Method
cpg	1223.29	J/mol×K	1032.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R59086&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