Docosane, 1,2-bis(methylthio)

Inchi: InChI=1S/C24H50S2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-24(26-3)2
InchiKey: FWSRWCPBZDYKSH-UHFFFAOYSA-N
Formula: C24H50S2
SMILES: CCCCCCCCCCCCCCCCCCCCC(CSC)SC
Mol. weight [g/mol]: 402.78

Physical Properties

Property code	Value	Unit	Source
gf	215.00	kJ/mol	Joback Method
hf	-460.23	kJ/mol	Joback Method
hfus	62.65	kJ/mol	Joback Method
hvap	82.26	kJ/mol	Joback Method
log10ws	-9.75		Crippen Method
logp	9.513		Crippen Method
mcvol	381.720	ml/mol	McGowan Method
pc	825.74	kPa	Joback Method
rinpol	3006.00		NIST Webbook
rinpol	3006.00		NIST Webbook
tb	885.64	K	Joback Method
tc	1084.91	K	Joback Method
tf	414.04	K	Joback Method
vc	1.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1243.64	J/mol×K	885.64	Joback Method
cpg	1264.86	J/mol×K	918.85	Joback Method
cpg	1284.76	J/mol×K	952.06	Joback Method
cpg	1303.37	J/mol×K	985.28	Joback Method
cpg	1320.76	J/mol×K	1018.49	Joback Method
cpg	1336.96	J/mol×K	1051.70	Joback Method
cpg	1352.03	J/mol×K	1084.91	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R59068&Units=SI

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