Tricosane, 1,2-bis(methylthio)

Inchi: InChI=1S/C25H52S2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-25(27-
InchiKey: FQDOMDIDSWOZGJ-UHFFFAOYSA-N
Formula: C25H52S2
SMILES: CCCCCCCCCCCCCCCCCCCCCCC(CSC)SC
Mol. weight [g/mol]: 416.81

Physical Properties

Property code	Value	Unit	Source
gf	223.42	kJ/mol	Joback Method
hf	-480.87	kJ/mol	Joback Method
hfus	65.24	kJ/mol	Joback Method
hvap	84.49	kJ/mol	Joback Method
log10ws	-10.17		Crippen Method
logp	9.903		Crippen Method
mcvol	395.810	ml/mol	McGowan Method
pc	782.00	kPa	Joback Method
rinpol	3107.00		NIST Webbook
tb	908.52	K	Joback Method
tc	1112.30	K	Joback Method
tf	425.31	K	Joback Method
vc	1.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1307.83	J/mol×K	908.52	Joback Method
cpg	1329.42	J/mol×K	942.48	Joback Method
cpg	1349.61	J/mol×K	976.45	Joback Method
cpg	1368.46	J/mol×K	1010.41	Joback Method
cpg	1386.01	J/mol×K	1044.37	Joback Method
cpg	1402.33	J/mol×K	1078.33	Joback Method
cpg	1417.46	J/mol×K	1112.30	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=R59353&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