Nonane, 2,3-bis-(methylthio), erythro

Inchi: InChI=1S/C11H24S2/c1-5-6-7-8-9-11(13-4)10(2)12-3/h10-11H,5-9H2,1-4H3/t10-,11+/m1
InchiKey: XTCRGULHQLHBIO-MNOVXSKESA-N
Formula: C11H24S2
SMILES: CCCCCCC(SC)C(C)SC
Mol. weight [g/mol]: 220.44

Physical Properties

Property code	Value	Unit	Source
gf	103.10	kJ/mol	Joback Method
hf	-197.19	kJ/mol	Joback Method
hfus	25.46	kJ/mol	Joback Method
hvap	52.94	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	4.440		Crippen Method
mcvol	198.550	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	1584.00		NIST Webbook
tb	587.76	K	Joback Method
tc	793.00	K	Joback Method
tf	252.53	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.51	J/mol×K	587.76	Joback Method
cpg	503.08	J/mol×K	621.97	Joback Method
cpg	519.75	J/mol×K	656.17	Joback Method
cpg	535.55	J/mol×K	690.38	Joback Method
cpg	550.48	J/mol×K	724.59	Joback Method
cpg	564.56	J/mol×K	758.80	Joback Method
cpg	577.81	J/mol×K	793.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R121801&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