Hexacosane, 1,2-bis(methylthio)

Inchi: InChI=1S/C28H58S2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25-
InchiKey: NSICRTSHVHWNQQ-UHFFFAOYSA-N
Formula: C28H58S2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCC(CSC)SC
Mol. weight [g/mol]: 458.89

Physical Properties

Property code	Value	Unit	Source
gf	248.68	kJ/mol	Joback Method
hf	-542.79	kJ/mol	Joback Method
hfus	73.01	kJ/mol	Joback Method
hvap	91.17	kJ/mol	Joback Method
log10ws	-11.42		Crippen Method
logp	11.073		Crippen Method
mcvol	438.080	ml/mol	McGowan Method
pc	669.77	kPa	Joback Method
rinpol	3425.00		NIST Webbook
tb	977.16	K	Joback Method
tc	1200.54	K	Joback Method
tf	459.12	K	Joback Method
vc	1.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1503.26	J/mol×K	977.16	Joback Method
cpg	1526.29	J/mol×K	1014.39	Joback Method
cpg	1547.62	J/mol×K	1051.62	Joback Method
cpg	1567.33	J/mol×K	1088.85	Joback Method
cpg	1585.51	J/mol×K	1126.08	Joback Method
cpg	1602.25	J/mol×K	1163.31	Joback Method
cpg	1617.61	J/mol×K	1200.54	Joback Method

Sources

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=R59139&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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