

Nonacosane, 1,2-bis(methylthio)

Inchi:	InChI=1S/C31H64S2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25
InchiKey:	KRQSDOFHULILLQ-UHFFFAOYSA-N
Formula:	C31H64S2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCC(CSC)SC
Mol. weight [g/mol]:	500.97

Physical Properties

Property code	Value	Unit	Source
gf	273.94	kJ/mol	Joback Method
hf	-604.71	kJ/mol	Joback Method
hfus	80.78	kJ/mol	Joback Method
hvap	97.85	kJ/mol	Joback Method
log10ws	-12.68		Crippen Method
logp	12.244		Crippen Method
mvol	480.350	ml/mol	McGowan Method
pc	580.08	kPa	Joback Method
rinpol	3726.00		NIST Webbook
rinpol	3726.00		NIST Webbook
tb	1045.80	K	Joback Method
tc	1299.71	K	Joback Method
tf	492.93	K	Joback Method
vc	1.873	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1702.06	J/mol×K	1045.80	Joback Method
cpg	1727.11	J/mol×K	1088.12	Joback Method
cpg	1750.01	J/mol×K	1130.44	Joback Method
cpg	1770.90	J/mol×K	1172.76	Joback Method
cpg	1789.92	J/mol×K	1215.07	Joback Method
cpg	1807.21	J/mol×K	1257.39	Joback Method
cpg	1822.90	J/mol×K	1299.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R59296&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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