

Hexane, 1,1'-thiobis-

Other names:	7-Thiatridecane Di-n-hexyl sulfide Dihexyl sulfide Hexyl sulfide Normal-hexyl sulfide dihexyl sulphide n-Hexyl sulfide
Inchi:	InChI=1S/C12H26S/c1-3-5-7-9-11-13-12-10-8-6-4-2/h3-12H2,1-2H3
InchiKey:	LHNRHYOMDUJLLM-UHFFFAOYSA-N
Formula:	C12H26S
SMILES:	CCCCCSCCCCC
Mol. weight [g/mol]:	202.40
CAS:	6294-31-1

Physical Properties

Property code	Value	Unit	Source
gf	83.28	kJ/mol	Joback Method
hf	-249.14	kJ/mol	Joback Method
hfus	30.97	kJ/mol	Joback Method
hvap	49.12	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.880		Crippen Method
mcvol	196.290	ml/mol	McGowan Method
pc	1806.16	kPa	Joback Method
rinpol	1468.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1499.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1473.00		NIST Webbook
ripol	1667.00		NIST Webbook
ripol	1667.00		NIST Webbook

ripol	1678.00		NIST Webbook
tb	503.20	K	NIST Webbook
tc	721.16	K	Joback Method
tf	259.40	K	Joback Method
vc	0.761	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.47	J/mol×K	691.42	Joback Method
cpg	472.53	J/mol×K	542.74	Joback Method
cpg	489.74	J/mol×K	572.48	Joback Method
cpg	506.22	J/mol×K	602.21	Joback Method
cpg	521.99	J/mol×K	631.95	Joback Method
cpg	537.07	J/mol×K	661.69	Joback Method
cpg	565.21	J/mol×K	721.16	Joback Method
hvapt	72.40	kJ/mol	373.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49517e+01
Coeff. B	-4.36250e+03
Coeff. C	-8.10260e+01
Temperature range (K), min.	378.52
Temperature range (K), max.	533.55

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=C6294311&Units=SI>

The Yaws Handbook of Vapor Pressure:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.cheméo.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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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