

di-n-Nonyl sulfide

Other names:	diNonyl sulfide diNonyl sulphide
Inchi:	InChI=1S/C18H38S/c1-3-5-7-9-11-13-15-17-19-18-16-14-12-10-8-6-4-2/h3-18H2,1-2H3
InchiKey:	KMKSVAGOBVUFRO-UHFFFAOYSA-N
Formula:	C18H38S
SMILES:	CCCCCCCCCSCCCCCCCCC
Mol. weight [g/mol]:	286.56
CAS:	929-98-6

Physical Properties

Property code	Value	Unit	Source
gf	133.80	kJ/mol	Joback Method
hf	-372.98	kJ/mol	Joback Method
hfus	46.51	kJ/mol	Joback Method
hvap	62.48	kJ/mol	Joback Method
log10ws	-7.24		Crippen Method
logp	7.221		Crippen Method
mcvol	280.830	ml/mol	McGowan Method
pc	1165.63	kPa	Joback Method
rinpol	2091.00		NIST Webbook
rinpol	2068.00		NIST Webbook
rinpol	2091.00		NIST Webbook
rinpol	2089.00		NIST Webbook
rinpol	2068.00		NIST Webbook
tb	680.02	K	Joback Method
tc	853.00	K	Joback Method
tf	327.02	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.70	J/molxK	680.02	Joback Method
cpg	819.62	J/molxK	708.85	Joback Method

cpg	838.64	J/mol×K	737.68	Joback Method
cpg	856.78	J/mol×K	766.51	Joback Method
cpg	874.07	J/mol×K	795.34	Joback Method
cpg	890.54	J/mol×K	824.17	Joback Method
cpg	906.20	J/mol×K	853.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C929986&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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