Undecyl sulfide

Other names:	1-(Undecylsulfanyl)undecane
	Diundecyl sulfide
	Undecane, 1-(undecylthio)-
Inchi:	InChI=1S/C22H46S/c1-3-5-7-9-11-13-15-17-19-21-23-22-20-18-16-14-12-10-8-6-4-2/h3-
InchiKey:	RDOYGXODZMRGKD-UHFFFAOYSA-N
Formula:	C22H46S
SMILES:	CCCCCCCCCCCSCCCCCCCCCC
Mol. weight [g/mol]:	342.67
CAS:	35599-82-7

Physical Properties

Property code	Value	Unit	Source
gf	167.48	kJ/mol	Joback Method
hf	-455.54	kJ/mol	Joback Method
hfus	56.87	kJ/mol	Joback Method
hvap	71.38	kJ/mol	Joback Method
log10ws	-8.92		Crippen Method
logp	8.781		Crippen Method
mcvol	337.190	ml/mol	McGowan Method
pc	911.08	kPa	Joback Method
rinpol	2481.00		NIST Webbook
rinpol	2481.00		NIST Webbook
tb	771.54	K	Joback Method
tc	949.40	K	Joback Method
tf	372.10	K	Joback Method
vc	1.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1041.74	J/mol×K	771.54	Joback Method
cpg	1063.09	J/mol×K	801.18	Joback Method
cpg	1083.40	J/mol×K	830.83	Joback Method
cpg	1102.69	J/mol×K	860.47	Joback Method

cpg	1121.00	J/mol×K	890.11	Joback Method
cpg	1138.37	J/mol×K	919.76	Joback Method
cpg	1154.83	J/mol×K	949.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35599827&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