

N-Decyl ethyl sulfide

Other names:	3-Thiatridecane
Inchi:	InChI=1S/C12H26S/c1-3-5-6-7-8-9-10-11-12-13-4-2/h3-12H2,1-2H3
InchiKey:	VSSRSPLEFYQIEK-UHFFFAOYSA-N
Formula:	C12H26S
SMILES:	CCCCCCCCCCCCSCC
Mol. weight [g/mol]:	202.40
CAS:	19313-61-2

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	1493.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1493.00		NIST Webbook
ripol	1710.00		NIST Webbook
ripol	1710.00		NIST Webbook
tb	542.74	K	Joback Method
tc	721.16	K	Joback Method
tf	259.40	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	551.47	J/mol×K	691.42	Joback Method
cpg	565.21	J/mol×K	721.16	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.61036e+01
Coeff. B	-4.97854e+03
Coeff. C	-9.02300e+01
Temperature range (K), min.	405.01
Temperature range (K), max.	551.54

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343410&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
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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