

3-Thiadecane

Other names:	ethyl heptyl sulfide heptyl ethyl sulfide
Inchi:	InChI=1S/C9H20S/c1-3-5-6-7-8-9-10-4-2/h3-9H2,1-2H3
InchiKey:	PYPULUCCVXMPFP-UHFFFAOYSA-N
Formula:	C9H20S
SMILES:	CCCCCCCCSCC
Mol. weight [g/mol]:	160.32
CAS:	24768-44-3

Physical Properties

Property code	Value	Unit	Source
gf	58.02	kJ/mol	Joback Method
hf	-187.22	kJ/mol	Joback Method
hfus	23.20	kJ/mol	Joback Method
hvap	42.45	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.710		Crippen Method
mcvol	154.020	ml/mol	McGowan Method
pc	2345.09	kPa	Joback Method
rinpol	1193.00		NIST Webbook
rinpol	1193.00		NIST Webbook
ripol	1411.00		NIST Webbook
ripol	1385.30		NIST Webbook
ripol	1390.70		NIST Webbook
tb	474.10	K	Joback Method
tc	657.88	K	Joback Method
tf	225.59	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.44	J/mol×K	474.10	Joback Method
cpg	345.32	J/mol×K	504.73	Joback Method

cpg	359.59	J/mol×K	535.36	Joback Method
cpg	373.27	J/mol×K	565.99	Joback Method
cpg	386.37	J/mol×K	596.62	Joback Method
cpg	398.90	J/mol×K	627.25	Joback Method
cpg	410.88	J/mol×K	657.88	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.60665e+01
Coeff. B	-4.51549e+03
Coeff. C	-7.49960e+01
Temperature range (K), min.	361.17
Temperature range (K), max.	494.84

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R140659&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/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
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

Latest version available from:

<https://www.cheméo.com/cid/14-079-9/3-Thiadecane.pdf>

Generated by Cheméo on 2025-12-23 02:31:18.126167448 +0000 UTC m=+6205275.656208131.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.