hexyl propyl sulfide

Other names:	4-Thiadecane
	Hexane, 1-(propylthio)-
Inchi:	InChI=1S/C9H20S/c1-3-5-6-7-9-10-8-4-2/h3-9H2,1-2H3
InchiKey:	ABZLKKGJOVPBBL-UHFFFAOYSA-N
Formula:	C9H20S
SMILES:	CCCCCCSCCC
Mol. weight [g/mol]:	160.32
CAS:	24768-43-2

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	1182.00		NIST Webbook
rinpol	1182.00		NIST Webbook
ripol	1372.00		NIST Webbook
ripol	1393.00		NIST Webbook
ripol	1372.00		NIST Webbook
ripol	1367.00		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(Pvp) = A + B/(T + C)
Coeff. A	1.59618e+01
Coeff. B	-4.47734e+03
Coeff. C	-7.47180e+01
Temperature range (K), min.	360.37
Temperature range (K), max.	495.11

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24768432&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

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