

heptyl propyl sulfide

Other names:	4-Thiaundecane
Inchi:	InChI=1S/C10H22S/c1-3-5-6-7-8-10-11-9-4-2/h3-10H2,1-2H3
InchiKey:	PCPVCHFVKVPNTBH-UHFFFAOYSA-N
Formula:	C10H22S
SMILES:	CCCCCCCCSCCC
Mol. weight [g/mol]:	174.35
CAS:	24768-46-5

Physical Properties

Property code	Value	Unit	Source
gf	66.44	kJ/mol	Joback Method
hf	-207.86	kJ/mol	Joback Method
hfus	25.79	kJ/mol	Joback Method
hvap	44.67	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	4.100		Crippen Method
mcvol	168.110	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinpol	1282.00		NIST Webbook
rinpol	1282.00		NIST Webbook
ripol	1470.30		NIST Webbook
ripol	1465.20		NIST Webbook
ripol	1492.00		NIST Webbook
tb	496.98	K	Joback Method
tc	678.93	K	Joback Method
tf	236.86	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.94	J/mol×K	496.98	Joback Method
cpg	391.70	J/mol×K	527.30	Joback Method
cpg	406.81	J/mol×K	557.63	Joback Method

cpg	421.28	J/mol×K	587.95	Joback Method
cpg	435.13	J/mol×K	618.28	Joback Method
cpg	448.38	J/mol×K	648.60	Joback Method
cpg	461.02	J/mol×K	678.93	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.64792e+01
Coeff. B	-4.82867e+03
Coeff. C	-8.14120e+01
Temperature range (K), min.	379.63
Temperature range (K), max.	513.79

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R140699&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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