

5-Thiaundecane

Other names:	butyl hexyl sulfide hexyl butyl sulfide
Inchi:	InChI=1S/C10H22S/c1-3-5-7-8-10-11-9-6-4-2/h3-10H2,1-2H3
InchiKey:	YZUHMAFUXBPUKH-UHFFFAOYSA-N
Formula:	C10H22S
SMILES:	CCCCCSCCCC
Mol. weight [g/mol]:	174.35
CAS:	16967-04-7

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	1278.00		NIST Webbook
rinpol	1278.00		NIST Webbook
ripol	1457.80		NIST Webbook
ripol	1463.80		NIST Webbook
ripol	1485.00		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	1.63721e+01
Coeff. B	-4.78833e+03
Coeff. C	-8.11340e+01
Temperature range (K), min.	378.83
Temperature range (K), max.	514.05

Sources

The Yaws Handbook of Vapor Pressure: Crippen Method:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://link.springer.com/article/10.1007/BF02311772
	http://webbook.nist.gov/cgi/cbook.cgi?ID=R140624&Units=SI

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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