

Thiepane

Other names:	Hexamethylene sulfide Thiacycloheptane Thiepin, hexahydro-
Inchi:	InChI=1S/C6H12S/c1-2-4-6-7-5-3-1/h1-6H2
InchiKey:	JWCVYQRPINPYQJ-UHFFFAOYSA-N
Formula:	C6H12S
SMILES:	C1CCCCSC1
Mol. weight [g/mol]:	116.22
CAS:	4753-80-4

Physical Properties

Property code	Value	Unit	Source
chl	-4565.25	kJ/mol	NIST Webbook
gf	59.56	kJ/mol	Joback Method
hf	-53.41	kJ/mol	Joback Method
hfl	-113.00 ± 2.00	kJ/mol	NIST Webbook
hfus	3.62	kJ/mol	Joback Method
hvap	35.67	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.294		Crippen Method
mcvol	100.890	ml/mol	McGowan Method
pc	4233.04	kPa	Joback Method
rinpol	963.00		NIST Webbook
rinpol	963.00		NIST Webbook
tb	446.70	K	NIST Webbook
tc	645.41	K	Joback Method
tf	248.93	K	Joback Method
vc	0.344	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.19	J/mol×K	413.00	Joback Method
cpg	194.25	J/mol×K	451.74	Joback Method

cpg	209.40	J/mol×K	490.47	Joback Method
cpg	223.64	J/mol×K	529.21	Joback Method
cpg	237.02	J/mol×K	567.94	Joback Method
cpg	249.56	J/mol×K	606.68	Joback Method
cpg	261.28	J/mol×K	645.41	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.62592e+01
Coeff. B	-1.98684e+04
Coeff. C	4.71396e+02
Temperature range (K), min.	293.61
Temperature range (K), max.	477.08

Sources

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=C4753804&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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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