

thiacyclodecane

Inchi:	InChI=1S/C9H18S/c1-2-4-6-8-10-9-7-5-3-1/h1-9H2
InchiKey:	IKUFHMODDAEPRX-UHFFFAOYSA-N
Formula:	C9H18S
SMILES:	C1CCCCSCCCC1
Mol. weight [g/mol]:	158.30
CAS:	6048-83-5

Physical Properties

Property code	Value	Unit	Source
af	0.1906		Cheméo Relay (1.0)
hf	-171.69	kJ/mol	Cheméo Relay (1.0)
hfus	5.09	kJ/mol	Joback Method
hvap	57.65	kJ/mol	Cheméo Relay (1.0)
ie	8.31	eV	Cheméo Relay (1.0)
logp	3.464		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
tb	505.27	K	Cheméo Relay (1.0)
tc	740.76	K	Cheméo Relay (1.0)
tf	308.73	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.09	J/mol×K	494.45	Joback Method
cpg	330.13	J/mol×K	536.11	Joback Method
cpg	351.79	J/mol×K	577.76	Joback Method
cpg	372.07	J/mol×K	619.42	Joback Method
cpg	390.99	J/mol×K	661.07	Joback Method
cpg	408.56	J/mol×K	702.73	Joback Method
cpg	424.78	J/mol×K	744.39	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.33927e+01
Coeff. B	-3.83463e+03
Coeff. C	-7.95600e+01
Temperature range (K), min.	372.16
Temperature range (K), max.	554.07

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6048835&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

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