

1,4,7,10-Tetrathiacyclododecane

Inchi:	InChI=1S/C8H16S4/c1-2-10-5-6-12-8-7-11-4-3-9-1/h1-8H2
InchiKey:	MULBAFLKPUVJKC-UHFFFAOYSA-N
Formula:	C8H16S4
SMILES:	C1CSCCSCCSCCS1
Mol. weight [g/mol]:	240.47
CAS:	25423-56-7

Physical Properties

Property code	Value	Unit	Source
gf	135.48	kJ/mol	Joback Method
hf	10.29	kJ/mol	Joback Method
hfus	9.27	kJ/mol	Joback Method
hvap	58.42	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.933		Crippen Method
mcvol	178.120	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
tb	623.60	K	Joback Method
tc	943.62	K	Joback Method
tf	504.22	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.34	J/mol×K	890.28	Joback Method
cpg	410.34	J/mol×K	623.60	Joback Method
cpg	433.62	J/mol×K	676.94	Joback Method
cpg	454.68	J/mol×K	730.27	Joback Method
cpg	473.49	J/mol×K	783.61	Joback Method
cpg	490.06	J/mol×K	836.95	Joback Method
cpg	516.32	J/mol×K	943.62	Joback Method
hfust	31.00	kJ/mol	499.20	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	434.20	K	0.07	NIST Webbook

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25423567&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
hfust:	Enthalpy of fusion at a given temperature
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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