

2,4,5,7,9-pentathiadecane

Inchi:	InChI=1S/C5H12S5/c1-6-3-8-5-10-9-4-7-2/h3-5H2,1-2H3
InchiKey:	BZFNKFPFLHCSC-UHFFFAOYSA-N
Formula:	C5H12S5
SMILES:	CSCSCSSCSC
Mol. weight [g/mol]:	232.47

Physical Properties

Property code	Value	Unit	Source
gf	156.82	kJ/mol	Joback Method
hf	62.82	kJ/mol	Joback Method
hfus	29.36	kJ/mol	Joback Method
hvap	60.81	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.700		Crippen Method
mcvol	163.060	ml/mol	McGowan Method
pc	3843.54	kPa	Joback Method
rinpol	1777.00		NIST Webbook
tb	657.70	K	Joback Method
tc	936.23	K	Joback Method
tf	318.11	K	Joback Method
vc	0.586	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.89	J/mol×K	657.70	Joback Method
cpg	359.04	J/mol×K	704.12	Joback Method
cpg	370.17	J/mol×K	750.54	Joback Method
cpg	380.22	J/mol×K	796.97	Joback Method
cpg	389.15	J/mol×K	843.39	Joback Method
cpg	396.89	J/mol×K	889.81	Joback Method
cpg	403.40	J/mol×K	936.23	Joback Method

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=R226392&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
mccvol:	McGowan's characteristic volume
pc:	Critical 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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