trans-1,2,3,4,4a,9a-Hexahydrodibenzothiophene

Inchi: InChI=1S/C12H14S/c1-3-7-11-9(5-1)10-6-2-4-8-12(10)13-11/h1,3,5,7,10,12H,2,4,6,8H2
InchiKey: VKFAAUDUBPEOMC-UHFFFAOYSA-N
Formula: C12H14S
SMILES: c1ccc2c(c1)SC1CCCCC21
Mol. weight [g/mol]: 190.31

Physical Properties

Property code	Value	Unit	Source
hfus	18.32	kJ/mol	Joback Method
logp	3.819		Crippen Method
mcvol	150.810	ml/mol	McGowan Method
rinpol	269.67		NIST Webbook

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-1.11410e+02
Coeff. B	1.31201e+00
Coeff. C	-1.00586e-03
Coeff. D	3.09700e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R15397&Units=SI

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):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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