Dibenzothiophene, 1,2,3,4-tetrahydro-

Other names: 1,2,3,4-Tetrahydrodibenzo[b,d]thiophene
1,2,3,4-tetrahydrodibenzothiophene
Tetrahydrodibenzothiophene
Inchi: InChI=1S/C12H12S/c1-3-7-11-9(5-1)10-6-2-4-8-12(10)13-11/h1,3,5,7H,2,4,6,8H2
InchiKey: JCLPOPNXITXHOR-UHFFFAOYSA-N
Formula: C12H12S
SMILES: c1ccc2c3c(sc2c1)CCCC3
Mol. weight [g/mol]: 188.29
CAS: 16587-33-0

Physical Properties

Property code	Value	Unit	Source
hfus	14.01	kJ/mol	Possible precursors and products of deep hydrodesulfurization of gasoline and distillate fuels III. The thermodynamic properties of 1,2,3,4-tetrahydrodibenzothiophene
hvap	75.30 ± 0.70	kJ/mol	NIST Webbook
log10ws	-4.53		Crippen Method
logp	3.780		Crippen Method
mcvol	146.510	ml/mol	McGowan Method
rinpol	294.30		NIST Webbook
rinpol	294.30		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	32.03	kJ/mol	275.00	NIST Webbook
hvapt	67.30 ± 0.30	kJ/mol	480.00	NIST Webbook
hvapt	64.50 ± 0.20	kJ/mol	480.00	NIST Webbook
hvapt	61.80 ± 0.20	kJ/mol	480.00	NIST Webbook
hvapt	59.20 ± 0.30	kJ/mol	480.00	NIST Webbook
hvapt	56.50 ± 0.40	kJ/mol	480.00	NIST Webbook
hvapt	70.30 ± 0.30	kJ/mol	480.00	NIST Webbook

Sources

Possible precursors and products of deep hydrodesulfurization of gasoline and distillate fuels III. The thermodynamic properties of 1,2,3,4-tetrahydrodibenzothiophene:	https://www.doi.org/10.1016/j.jct.2003.12.012
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16587330&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices