Dibenzo[b,f]thiepin

Inchi: InChI=1S/C14H10S/c1-3-7-13-11(5-1)9-10-12-6-2-4-8-14(12)15-13/h1-10H
InchiKey: KMAWVRYYKYVCNR-UHFFFAOYSA-N
Formula: C14H10S
SMILES: C1=Cc2ccccc2Sc2ccccc21
Mol. weight [g/mol]: 210.29
CAS: 257-13-6

Physical Properties

Property code	Value	Unit	Source
gf	410.84	kJ/mol	Joback Method
hf	314.01	kJ/mol	Joback Method
hfus	21.26	kJ/mol	Joback Method
hvap	58.96	kJ/mol	Joback Method
ie	7.96	eV	NIST Webbook
log10ws	-4.74		Crippen Method
logp	4.322		Crippen Method
mcvol	161.790	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
tb	641.44	K	Joback Method
tc	916.01	K	Joback Method
tf	431.81	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.97	J/mol×K	641.44	Joback Method
cpg	392.94	J/mol×K	687.20	Joback Method
cpg	406.51	J/mol×K	732.96	Joback Method
cpg	418.84	J/mol×K	778.73	Joback Method
cpg	430.12	J/mol×K	824.49	Joback Method
cpg	440.50	J/mol×K	870.25	Joback Method
cpg	450.16	J/mol×K	916.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C257136&Units=SI
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

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
ie:	Ionization energy
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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