Hydantoin, 5,5-bis[(benzylthio)methyl]-

Inchi: InChI=1S/C19H20N2O2S2/c22-17-19(21-18(23)20-17,13-24-11-15-7-3-1-4-8-15)14-25-1
InchiKey: JCDRJBAHSISSAL-UHFFFAOYSA-N
Formula: C19H20N2O2S2
SMILES: O=C1NC(=O)C(CSCc2ccccc2)(CSCc2ccccc2)N1
Mol. weight [g/mol]: 372.50
CAS: 32418-95-4

Physical Properties

Property code	Value	Unit	Source
gf	361.46	kJ/mol	Joback Method
hf	-2.75	kJ/mol	Joback Method
hfus	47.14	kJ/mol	Joback Method
hvap	97.19	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	3.431		Crippen Method
mcvol	275.990	ml/mol	McGowan Method
pc	2497.50	kPa	Joback Method
tb	1073.30	K	Joback Method
tc	1371.81	K	Joback Method
tf	806.83	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	893.79	J/mol×K	1073.30	Joback Method
cpg	910.60	J/mol×K	1123.05	Joback Method
cpg	926.53	J/mol×K	1172.80	Joback Method
cpg	941.76	J/mol×K	1222.56	Joback Method
cpg	956.48	J/mol×K	1272.31	Joback Method
cpg	970.89	J/mol×K	1322.06	Joback Method
cpg	985.17	J/mol×K	1371.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32418954&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
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