5,5-diethyl-2-sulfanylidene-1,3-diazinane-4,6-dion

Inchi: InChI=1S/C8H12N2O2S/c1-3-8(4-2)5(11)9-7(13)10-6(8)12/h3-4H2,1-2H3,(H2,9,10,11,12
InchiKey: QGVNJRROSLYGKF-UHFFFAOYSA-N
Formula: C8H12N2O2S
SMILES: CCC1(CC)C(=O)NC(=S)NC1=O
Mol. weight [g/mol]: 200.26

Physical Properties

Property code	Value	Unit	Source
gf	56.53	kJ/mol	Joback Method
hf	-223.57	kJ/mol	Joback Method
hfus	26.25	kJ/mol	Joback Method
hvap	62.17	kJ/mol	Joback Method
log10ws	-2.32		Aqueous Solubility Prediction Method
logp	0.324		Crippen Method
mcvol	147.870	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
tb	707.61	K	Joback Method
tc	976.26	K	Joback Method
tf	621.37	K	Joback Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.29	J/mol×K	707.61	Joback Method
cpg	403.21	J/mol×K	752.39	Joback Method
cpg	417.51	J/mol×K	797.16	Joback Method
cpg	431.28	J/mol×K	841.94	Joback Method
cpg	444.61	J/mol×K	886.71	Joback Method
cpg	457.58	J/mol×K	931.49	Joback Method
cpg	470.28	J/mol×K	976.26	Joback Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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