5-methyl-5-propyl-1,3-diazinane-2,4,6-trione

Inchi: InChI=1S/C8H12N2O3/c1-3-4-8(2)5(11)9-7(13)10-6(8)12/h3-4H2,1-2H3,(H2,9,10,11,12,1
InchiKey: KWEHOVAGMBSHNZ-UHFFFAOYSA-N
Formula: C8H12N2O3
SMILES: CCCC1(C)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 184.20

Physical Properties

Property code	Value	Unit	Source
gf	-156.91	kJ/mol	Joback Method
hf	-476.37	kJ/mol	Joback Method
hfus	19.72	kJ/mol	Joback Method
hvap	58.94	kJ/mol	Joback Method
log10ws	-1.49		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	0.159		Crippen Method
mcvol	137.390	ml/mol	McGowan Method
pc	4000.70	kPa	Joback Method
tb	702.79	K	Joback Method
tc	967.84	K	Joback Method
tf	625.92	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.82	J/mol×K	702.79	Joback Method
cpg	404.44	J/mol×K	746.96	Joback Method
cpg	420.27	J/mol×K	791.14	Joback Method
cpg	435.31	J/mol×K	835.31	Joback Method
cpg	449.56	J/mol×K	879.49	Joback Method
cpg	462.99	J/mol×K	923.66	Joback Method
cpg	475.62	J/mol×K	967.84	Joback Method

Sources

Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
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