5-ethyl-1,3-diazinane-2,4,6-trione

Inchi: InChI=1S/C6H8N2O3/c1-2-3-4(9)7-6(11)8-5(3)10/h3H,2H2,1H3,(H2,7,8,9,10,11)
InchiKey: FMTLDVACNZDTQL-UHFFFAOYSA-N
Formula: C6H8N2O3
SMILES: CCC1C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 156.14

Physical Properties

Property code	Value	Unit	Source
gf	-168.26	kJ/mol	Joback Method
hf	-450.33	kJ/mol	Joback Method
hfus	20.84	kJ/mol	Joback Method
hvap	55.64	kJ/mol	Joback Method
log10ws	-1.43		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	-0.621		Crippen Method
mcvol	109.210	ml/mol	McGowan Method
pc	4862.97	kPa	Joback Method
tb	656.79	K	Joback Method
tc	924.45	K	Joback Method
tf	579.48	K	Joback Method
vc	0.400	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.48	J/mol×K	656.79	Joback Method
cpg	305.57	J/mol×K	701.40	Joback Method
cpg	319.73	J/mol×K	746.01	Joback Method
cpg	332.78	J/mol×K	790.62	Joback Method
cpg	344.53	J/mol×K	835.23	Joback Method
cpg	354.81	J/mol×K	879.84	Joback Method
cpg	363.43	J/mol×K	924.45	Joback Method

Sources

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

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