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

Inchi: InChI=1S/C13H22N2O3/c1-3-5-6-7-8-9-13(4-2)10(16)14-12(18)15-11(13)17/h3-9H2,1-2H
InchiKey: FLJQERBDKWFELA-UHFFFAOYSA-N
Formula: C13H22N2O3
SMILES: CCCCCCCC1(CC)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 254.33

Physical Properties

Property code	Value	Unit	Source
gf	-114.81	kJ/mol	Joback Method
hf	-579.57	kJ/mol	Joback Method
hfus	32.67	kJ/mol	Joback Method
hvap	70.07	kJ/mol	Joback Method
log10ws	-3.22		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	2.109		Crippen Method
mcvol	207.840	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
tb	817.19	K	Joback Method
tc	1055.63	K	Joback Method
tf	682.27	K	Joback Method
vc	0.789	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.69	J/mol×K	817.19	Joback Method
cpg	682.59	J/mol×K	856.93	Joback Method
cpg	700.46	J/mol×K	896.67	Joback Method
cpg	717.32	J/mol×K	936.41	Joback Method
cpg	733.19	J/mol×K	976.15	Joback Method
cpg	748.09	J/mol×K	1015.89	Joback Method
cpg	762.03	J/mol×K	1055.63	Joback Method

Sources

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/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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