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

Inchi: InChI=1S/C14H24N2O3/c1-3-5-6-7-8-9-10-14(4-2)11(17)15-13(19)16-12(14)18/h3-10H2
InchiKey: NTYYDJWPKCQQIB-UHFFFAOYSA-N
Formula: C14H24N2O3
SMILES: CCCCCCCCC1(CC)C(=O)NC(=O)NC1=O
Mol. weight [g/mol]: 268.36

Physical Properties

Property code	Value	Unit	Source
gf	-106.39	kJ/mol	Joback Method
hf	-600.21	kJ/mol	Joback Method
hfus	35.26	kJ/mol	Joback Method
hvap	72.29	kJ/mol	Joback Method
log10ws	-3.94		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	2.499		Crippen Method
mcvol	221.930	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
tb	840.07	K	Joback Method
tc	1074.84	K	Joback Method
tf	693.54	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	722.26	J/mol×K	840.07	Joback Method
cpg	741.38	J/mol×K	879.20	Joback Method
cpg	759.44	J/mol×K	918.33	Joback Method
cpg	776.47	J/mol×K	957.46	Joback Method
cpg	792.49	J/mol×K	996.59	Joback Method
cpg	807.51	J/mol×K	1035.71	Joback Method
cpg	821.56	J/mol×K	1074.84	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