N-cyclopropyl-3,4,5-tri-methoxybenzamide

Inchi: InChI=1S/C13H17NO4/c1-16-10-6-8(13(15)14-9-4-5-9)7-11(17-2)12(10)18-3/h6-7,9H,4-5
InchiKey: SJPYUSAXGYQKLM-UHFFFAOYSA-N
Formula: C13H17NO4
SMILES: COc1cc(C(=O)NC2CC2)cc(OC)c1OC
Mol. weight [g/mol]: 251.28
CAS: 92042-04-1

Physical Properties

Property code	Value	Unit	Source
gf	-151.68	kJ/mol	Joback Method
hf	-492.50	kJ/mol	Joback Method
hfus	30.70	kJ/mol	Joback Method
hvap	69.12	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	1.605		Crippen Method
mcvol	188.570	ml/mol	McGowan Method
pc	2438.65	kPa	Joback Method
tb	716.50	K	Joback Method
tc	930.60	K	Joback Method
tf	487.47	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.72	J/mol×K	716.50	Joback Method
cpg	547.29	J/mol×K	752.18	Joback Method
cpg	560.93	J/mol×K	787.87	Joback Method
cpg	573.67	J/mol×K	823.55	Joback Method
cpg	585.50	J/mol×K	859.23	Joback Method
cpg	596.43	J/mol×K	894.92	Joback Method
cpg	606.48	J/mol×K	930.60	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92042041&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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