Cyclobutanecarboxamide, N-(2,5-dimethoxyphenyl)-

Inchi: InChI=1S/C13H17NO3/c1-16-10-6-7-12(17-2)11(8-10)14-13(15)9-4-3-5-9/h6-9H,3-5H2,1

InchiKey: RJOFFLXFRCDEGY-UHFFFAOYSA-N

Formula: C13H17NO3

SMILES: COc1ccc(OC)c(NC(=O)C2CCC2)c1

Mol. weight [g/mol]: 235.28

Physical Properties

Property code	Value	Unit	Source
gf	-49.15	kJ/mol	Joback Method
hf	-354.97	kJ/mol	Joback Method
hfus	27.80	kJ/mol	Joback Method
hvap	66.22	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.442		Crippen Method
mcvol	182.700	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinpol	2024.00		NIST Webbook
rinpol	2024.00		NIST Webbook
tb	693.37	K	Joback Method
tc	915.32	K	Joback Method
tf	449.20	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.59	J/mol×K	693.37	Joback Method
cpg	525.34	J/mol×K	730.36	Joback Method
cpg	540.04	J/mol×K	767.35	Joback Method
cpg	553.71	J/mol×K	804.35	Joback Method
cpg	566.37	J/mol×K	841.34	Joback Method
cpg	578.05	J/mol×K	878.33	Joback Method
cpg	588.77	J/mol×K	915.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307051&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume