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

Inchi: InChI=1S/C12H15NO3/c1-15-9-5-6-11(16-2)10(7-9)13-12(14)8-3-4-8/h5-8H,3-4H2,1-2H3

InchiKey: IBCVYNJHZCKFIG-UHFFFAOYSA-N

Formula: C12H15NO3

SMILES: COc1ccc(OC)c(NC(=O)C2CC2)c1

Mol. weight [g/mol]: 221.25

Physical Properties

Property code	Value	Unit	Source
gf	-45.47	kJ/mol	Joback Method
hf	-328.17	kJ/mol	Joback Method
hfus	27.31	kJ/mol	Joback Method
hvap	63.82	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.052		Crippen Method
mcvol	168.610	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
rinpol	1924.00		NIST Webbook
tb	666.22	K	Joback Method
tc	885.29	K	Joback Method
tf	441.45	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.34	J/mol×K	666.22	Joback Method
cpg	469.89	J/mol×K	702.73	Joback Method
cpg	483.51	J/mol×K	739.24	Joback Method
cpg	496.23	J/mol×K	775.76	Joback Method
cpg	508.09	J/mol×K	812.27	Joback Method
cpg	519.11	J/mol×K	848.78	Joback Method
cpg	529.32	J/mol×K	885.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307190&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

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