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

Inchi: InChI=1S/C15H21NO3/c1-18-12-8-9-14(19-2)13(10-12)16-15(17)11-6-4-3-5-7-11/h8-11H

InchiKey: BVAITUYABNDCPN-UHFFFAOYSA-N

Formula: C15H21NO3

SMILES: COc1ccc(OC)c(NC(=O)C2CCCCC2)c1

Mol. weight [g/mol]: 263.33

Physical Properties

Property code	Value	Unit	Source
gf	-56.51	kJ/mol	Joback Method
hf	-408.57	kJ/mol	Joback Method
hfus	28.78	kJ/mol	Joback Method
hvap	71.02	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.223		Crippen Method
mcvol	210.880	ml/mol	McGowan Method
pc	2246.13	kPa	Joback Method
rinpol	2226.00		NIST Webbook
rinpol	2226.00		NIST Webbook
tb	747.67	K	Joback Method
tc	974.98	K	Joback Method
tf	464.70	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.00	J/mol×K	747.67	Joback Method
cpg	641.68	J/mol×K	785.56	Joback Method
cpg	658.00	J/mol×K	823.44	Joback Method
cpg	672.98	J/mol×K	861.33	Joback Method
cpg	686.63	J/mol×K	899.21	Joback Method
cpg	698.96	J/mol×K	937.10	Joback Method
cpg	709.99	J/mol×K	974.98	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306950&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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