1-Naphthalenecarboxamide, N-(2,5-dimethoxyphenyl)-

Inchi: InChI=1S/C19H17NO3/c1-22-14-10-11-18(23-2)17(12-14)20-19(21)16-9-5-7-13-6-3-4-8-
InchiKey: HZTWQBPZMLHFPW-UHFFFAOYSA-N
Formula: C19H17NO3
SMILES: COc1ccc(OC)c(NC(=O)c2cccc3ccccc23)c1
Mol. weight [g/mol]: 307.34

Physical Properties

Property code	Value	Unit	Source
gf	162.15	kJ/mol	Joback Method
hf	-129.32	kJ/mol	Joback Method
hfus	37.97	kJ/mol	Joback Method
hvap	84.07	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.109		Crippen Method
mcvol	234.880	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
rinpol	2820.00		NIST Webbook
rinpol	2820.00		NIST Webbook
tb	870.28	K	Joback Method
tc	1112.27	K	Joback Method
tf	574.04	K	Joback Method
vc	0.882	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	687.06	J/mol×K	870.28	Joback Method
cpg	700.31	J/mol×K	910.61	Joback Method
cpg	712.36	J/mol×K	950.94	Joback Method
cpg	723.29	J/mol×K	991.28	Joback Method
cpg	733.15	J/mol×K	1031.61	Joback Method
cpg	742.01	J/mol×K	1071.94	Joback Method
cpg	749.93	J/mol×K	1112.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307409&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