

2-Naphthalenecarboxamide, N-(5-chloro-2,4-dimethoxyphenyl)-3-hydroxy-

Other names:

Acco Naf-Sol AS-ITR
Acco Naphthol AS-ITR
Acna Naphthol SS
Amanil Naphthol AS-ITR
Azoground ITR
Azotol O
C.I. Azoic Coupling Component 12
C.I. 37550
Daito Grounder ITR
Hiltonaphthol AS-ITR
Naphtanilide ITR
Naphtazol STR
Naphthoide ITR
Naphthol AS-ITR
Naphtoelan JTR
Naphtol AS-ITR
Naphtol AS-ITRLL
Sanatol ITR
Solunaptol ITR
Ultrazol IX-ITR
2-Naphthanilide, 5'-chloro-3-hydroxy-2',4'-dimethoxy-
5'-Chloro-3-hydroxy-2',4'-dimethoxy-2-naphthanilide
NSC 50687

Inchi: InChI=1S/C19H16ClNO4/c1-24-17-10-18(25-2)15(9-14(17)20)21-19(23)13-7-11-5-3-4-6-

InchiKey: XDWATWCCUTYUDE-UHFFFAOYSA-N

Formula: C19H16ClNO4

SMILES: COc1cc(OC)c(NC(=O)c2cc3ccccc3cc2O)cc1Cl

Mol. weight [g/mol]: 357.79

CAS: 92-72-8

Physical Properties

Property code	Value	Unit	Source
gf	-14.03	kJ/mol	Joback Method
hf	-333.84	kJ/mol	Joback Method
hfus	47.56	kJ/mol	Joback Method
hvap	102.13	kJ/mol	Joback Method

log10ws	-5.72		Crippen Method
logp	4.468		Crippen Method
mcvol	252.990	ml/mol	McGowan Method
pc	2400.57	kPa	Joback Method
tb	993.31	K	Joback Method
tc	1245.42	K	Joback Method
tf	728.20	K	Joback Method
vc	0.897	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	751.24	J/mol×K	993.31	Joback Method
cpg	763.04	J/mol×K	1035.33	Joback Method
cpg	774.31	J/mol×K	1077.35	Joback Method
cpg	785.17	J/mol×K	1119.37	Joback Method
cpg	795.74	J/mol×K	1161.39	Joback Method
cpg	806.15	J/mol×K	1203.40	Joback Method
cpg	816.53	J/mol×K	1245.42	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=C92728&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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