

Naphtol-as-itr

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

Physical Properties

Property code	Value	Unit	Source
hfus	47.56	kJ/mol	Joback Method
logp	4.468		Crippen Method
mcvol	252.990	ml/mol	McGowan 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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C92728&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity

hfus: Enthalpy of fusion at standard conditions

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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