

Naphthol-as-bg

Other names:	Acna Naphthol BG
	Amanil Naphthol AS-BG
	Azoic Coupling Component 19
	Brenthol FO
	C.I. Azoic Coupling Component 19
	C.I. 37545
	Cibanaphthol RDM
	Daito Grounder BG
	Hiltonaphthol AS-BG
	Naphtanilide BG
	Naphtanilide BG Supra
	Naphtazol BJ
	Naphthol AS-BG
	Naphthol AS-BG Dispersible
	Naphthol AS-BG Supra
	Naphtol AS-BG
	Naphtol AS-BG Supra
	Sanatol BG
	Solunaptol FOL
	Tulathol AS BG
	2-Naphthanilide, 3-hydroxy-2',5'-dimethoxy-
	NSC 37618
	3-hydroxy-2',5'-dimethoxynaphthanilide
Inchi:	InChI=1S/C19H17NO4/c1-23-14-7-8-18(24-2)16(11-14)20-19(22)15-9-12-5-3-4-6-13(12)
InchiKey:	LAKNSQZHAUYJJM-UHFFFAOYSA-N
Formula:	C19H17NO4
SMILES:	COc1ccc(OC)c(NC(=O)c2cc3ccccc3cc2O)c1
Mol. weight [g/mol]:	323.35

Physical Properties

Property code	Value	Unit	Source
hf	-378.84	kJ/mol	Cheméo Relay (1.0)
hfus	43.76	kJ/mol	Joback Method
logp	3.815		Crippen Method
mcvol	240.750	ml/mol	McGowan Method
tb	711.19	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.08	J/mol×K	950.90	Joback Method
cpg	745.68	J/mol×K	992.35	Joback Method
cpg	757.63	J/mol×K	1033.80	Joback Method
cpg	769.08	J/mol×K	1075.24	Joback Method
cpg	780.13	J/mol×K	1116.69	Joback Method
cpg	790.92	J/mol×K	1158.14	Joback Method
cpg	801.57	J/mol×K	1199.59	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C92739&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

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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