

Nafronyl

Other names:	2-Furanpropanoic acid, tetrahydro-«alpha»-(1-naphthalenylmethyl)-, 2-(diethylamino)ethyl ester 2-Furanpropionic acid, tetrahydro-«alpha»-(1-naphthylmethyl)-, 2-(diethylamino)ethyl ester N-Diethylaminoethyl «beta»-(1-naphthyl)-«beta»-tetrahydrofuryl isobutyrate 2-(Diethylamino)ethyl tetrahydro-«alpha»-(1-naphthylmethyl)-2-furanpropionate Nafronyl 3-(1-Naphthyl)-2-tetrahydrofurfurylpropionic acid 2-(diethylamino)ethyl ester «alpha»-Tetrahydrofurfuryl-1-naphthalenepropionic acid 2-(diethylamino)ethyl ester Tetrahydro-«alpha»-(1-naphthalenylmethyl)-2-furanpropanoic acid 2-(diethylamino)ethyl ester Tetrahydro-«alpha»-(1-naphthylmethyl)-2-furanpropanoic acid 2-(diethylamino)ethyl ester Tindus 2-(Diethylamino)ethyl ester tetrahydro-«alpha»-(1-naphthalenylmethyl)-2-furanpropanic acid Gevatran 2-(Diethylamino)ethyl 3-(1-naphthyl)-2-(tetrahydro-2-furanylmethyl)propanoate 2-(Diethylamino)ethyl tetrahydro-«alpha»-(1-naphthylmethyl)-2-furanpropionate ester LS 84 Naphtidrofuryl
Inchi:	InChI=1S/C24H33NO3/c1-3-25(4-2)14-16-28-24(26)21(18-22-12-8-15-27-22)17-20-11-7-
InchiKey:	KBAFPSLPKGSANY-UHFFFAOYSA-N
Formula:	C24H33NO3
SMILES:	CCN(CC)CCOC(=O)C(Cc1cccc2ccccc12)CC1CCCO1
Mol. weight [g/mol]:	383.53

Physical Properties

Property code	Value	Unit	Source
hfus	52.79	kJ/mol	Joback Method
logp	4.453		Crippen Method
mcvol	318.230	ml/mol	McGowan Method
rinpol	2786.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.11	J/mol×K	929.68	Joback Method

cpg	1079.52	J/mol×K	966.81	Joback Method
cpg	1095.73	J/mol×K	1003.93	Joback Method
cpg	1110.84	J/mol×K	1041.06	Joback Method
cpg	1124.96	J/mol×K	1078.19	Joback Method
cpg	1138.20	J/mol×K	1115.31	Joback Method
cpg	1150.68	J/mol×K	1152.44	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31329574&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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