Naftidrofuryl

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
Tridus
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]: 383.52

CAS: 31329-57-4

Physical Properties

Property code	Value	Unit	Source
gf	185.48	kJ/mol	Joback Method
hf	-376.63	kJ/mol	Joback Method
hfus	52.79	kJ/mol	Joback Method
hvap	89.17	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	4.453		Crippen Method
mcvol	318.230	ml/mol	McGowan Method
pc	1333.93	kPa	Joback Method
rinpol	2786.00		NIST Webbook
rinpol	2786.00		NIST Webbook
tb	929.68	K	Joback Method
tc	1152.44	K	Joback Method

tf	558.98	K	Joback Method
vc	1.192	m3/kmol	Joback Method

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: https://www.chemeo.com/doc/models/crippen_log10ws
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=C31329574&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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