Cocaine

Other names:

8-Azabicyclo[3.2.1]octane-2-carboxylic acid, 3-(benzoyloxy)-8-methyl-, methyl ester, [1R-(exo,exo)]-
1«alpha»H,5«alpha»H-Tropane-2«beta»-carboxylic acid, 3«beta»-hydroxy-, methyl ester, benzoate (ester)
L-Cocaine
Benzoylmethylecgonine
Ecgonine, methyl ester, benzoate (ester)
Neurocaine
2«beta»-Carbomethoxy-3«beta»-benzoyloxytropane
2«beta»-Tropanecarboxylic acid, 3«beta»-hydroxy-, methyl ester, benzoate (ester)
1-«alpha»-H,5-«alpha»-H-Tropane-2-«beta»-carboxylic acid, 3-«beta»-hydroxy-, methyl ester, benzoate
Bernice
Bernies
Burese
Cecil
Cholly
Coke
Corine
Ecgonine, methyl ester, benzoate
Eritroxilina
Erytroxylin
Girl
Gold dust
Happy dust
Kokain
Kokan
Kokayeen
Methyl 3-«beta»-hydroxy-1-«alpha»-H,5-«alpha»-H-tropane-2-«beta»-carboxylate benzoate
Star dust
2-«beta»-Tropanecarboxylic acid, 3-«beta»-hydroxy-, methyl ester, benzoate
3-Tropanylbenzoate-2-carboxylic acid methyl ester
Methyl 3«beta»-hydroxy-1«alpha»H,5«alpha»H-tropane-2«beta»-carboxylate benzoate (ester)
3«beta»-Hydroxy-2«beta»-tropanecarboxylic acid methyl ester, benzoate
2-Methyl-3«beta»-hydroxy-1«alpha»H,5«alpha»H-tropane-2«beta»-carboxylate benzoate (ester)
(1R,2R,3S,5S)-2-Methoxycarbonyltropan-3-yl benzoate

Inchi: InChI=1S/C17H21NO4/c1-18-12-8-9-13(18)15(17(20)21-2)14(10-12)22-16(19)11-6-4-3-5

InchiKey: ZPUCINDJVBIVPJ-PFSRBDOWSA-N

Formula: C17H21NO4

SMILES: COC(=O)C1C(OC(=O)c2ccccc2)CC2CCC1N2C

Mol. weight [g/mol]: 303.35

CAS: 50-36-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.80		Crippen Method
logp	1.868		Crippen Method
mcvol	229.770	ml/mol	McGowan Method
rinpol	2233.00		NIST Webbook
rinpol	2184.00		NIST Webbook
rinpol	2185.00		NIST Webbook
rinpol	2177.00		NIST Webbook
rinpol	2200.00		NIST Webbook
rinpol	2235.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2191.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2186.00		NIST Webbook
rinpol	2175.00		NIST Webbook
rinpol	2176.00		NIST Webbook
rinpol	2175.00		NIST Webbook
rinpol	2161.00		NIST Webbook
rinpol	2190.00		NIST Webbook
rinpol	2179.00		NIST Webbook
rinpol	2187.00		NIST Webbook
rinpol	2187.00		NIST Webbook
rinpol	2187.00		NIST Webbook
rinpol	2163.00		NIST Webbook
rinpol	2161.00		NIST Webbook
rinpol	2175.00		NIST Webbook
rinpol	2176.00		NIST Webbook
rinpol	2190.00		NIST Webbook
rinpol	2187.00		NIST Webbook
rinpol	2187.00		NIST Webbook
rinpol	2182.00		NIST Webbook
rinpol	2179.00		NIST Webbook
rinpol	2179.00		NIST Webbook
rinpol	2179.00		NIST Webbook
rinpol	2178.00		NIST Webbook
rinpol	2178.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2182.00		NIST Webbook
rinpol	2179.00		NIST Webbook
rinpol	2180.00		NIST Webbook

rinpol	2233.00	NIST Webbook
rinpol	2187.00	NIST Webbook
rinpol	2186.00	NIST Webbook
rinpol	2190.00	NIST Webbook
rinpol	2187.00	NIST Webbook
rinpol	2175.00	NIST Webbook
rinpol	2179.00	NIST Webbook
rinpol	2191.00	NIST Webbook
rinpol	2177.00	NIST Webbook
rinpol	2235.00	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	112.30 ± 2.80	kJ/mol	304.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50362&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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