FLUTAMIDE

Other names:	4'-Nitro-3'-trifluoromethylisobutyranilide
	4-Nitro-3-(trifluoromethyl)isobutyranilide
	Cebatrol, veterinary
	Eulexin
	NFBA
	NSC 215876
	Niftholide
	Niftolide
	Propanamide, 2-methyl-N-[4-nitro-3-(trifluoromethyl)phenyl]-
	Sch 13521
	m-Propionotoluidide, 2-methyl-4'-nitro-«alpha»,«alpha»,«alpha»-trifluoro-
	m-Propionotoluidide, «alpha»,«alpha»,«alpha»-trifluoro-2-methyl-4'-nitro-
	«alpha»,«alpha»,«alpha»-Trifluoro-2-methyl-4'-nitro-m-propionotoluidide
Inchi:	InChI=1S/C11H11F3N2O3/c1-6(2)10(17)15-7-3-4-9(16(18)19)8(5-7)11(12,13)14/h3-6H,1
InchiKey:	MKXKFYHWDHIYRV-UHFFFAOYSA-N
Formula:	C11H11F3N2O3
SMILES:	CC(C)C(=O)Nc1ccc([N+](=O)[O-])c(C(F)(F)F)c1
Mol. weight [g/mol]:	276.21

Physical Properties

Property code	Value	Unit	Source
hfus	33.87	kJ/mol	Joback Method
logp	3.208		Crippen Method
mcvol	176.370	ml/mol	McGowan Method
tb	558.48	K	Cheméo Relay (1.0)
tf	384.00	K	Solubilities of Flutamide, Dutasteride, and Finasteride as Antiandrogenic Agents, in Supercritical Carbon Dioxide: Measurement and Correlation

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	495.80	J/mol×K	737.74	Joback Method
cpg	506.93	J/mol×K	774.73	Joback Method
cpg	517.15	J/mol×K	811.71	Joback Method
cpg	526.54	J/mol×K	848.70	Joback Method
cpg	535.16	J/mol×K	885.68	Joback Method
cpg	543.07	J/mol×K	922.67	Joback Method
cpg	550.33	J/mol×K	959.65	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Solubilities of Flutamide, Dutasteride, and Finasteride as Antiandrogenic Agents in Supercritical Carbon Dioxide: Measurement and Correlation:	https://www.doi.org/10.1021/je900520a
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13311847&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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point