BENOXAPROFEN

Other names:	5-Benzoxazoleacetic acid, 2-(4-chlorophenyl)-«alpha»-methyl- Compound 90459 Coxigon Inflamid Opren 2-(p-Chlorophenyl)-«alpha»-methyl-5-benzoxazoleacetic acid 2-(4-Chlorophenyl)-«alpha»-methyl-5-benzoxazoleacetic acid Oraflex Uniprofen 5-Benzoxazoleacetic acid, 2-(4-chlorophenyl)-«alpha»-methyl, (.+/-.)- (.+/-.)-2-(p-Chlorophenyl)-«alpha»-methyl-5-benzoxazoleacetic acid NSC 299582 Lilly 90459
Inchi:	InChI=1S/C16H12ClNO3/c1-9(16(19)20)11-4-7-14-13(8-11)18-15(21-14)10-2-5-12(17)6-
InchiKey:	MITFXPHMIHQXPI-UHFFFAOYSA-N
Formula:	C16H12ClNO3
SMILES:	CC(C(=O)O)c1ccc2oc(-c3ccc(Cl)cc3)nc2c1
Mol. weight [g/mol]:	301.73

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.30		Cheméo Relay (1.0)
logp	4.336		Crippen Method
mcvol	209.150	ml/mol	McGowan Method
tf	417.15	K	Cheméo Relay (1.0)

Sources

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=C51234287&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point