

Enrofloxacin

Other names:

1-cyclopropyl-6-fluoro-7-(4-ethyl-1-piperazinyl)-1,4-dihydro-4-oxo-3-quinolinecarboxylic acid

Inchi:

1-cyclopropyl-7-(4-ethylpiperazin-1-yl)-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid

InchiKey:

SPFYMRJSYKOXGV-UHFFFAOYSA-N

Formula:

C19H22FN3O3

SMILES:

CCN1CCN(c2cc3c(cc2F)c(=O)c(C(=O)O)cn3C2CC2)CC1

Mol. weight [g/mol]:

359.40

Physical Properties

Property code	Value	Unit	Source
hfus	32.90	kJ/mol	Sublimation thermodynamics of four fluoroquinolone antimicrobial compounds
log10ws	-3.68		Crippen Method
logp	2.316		Crippen Method
mcvol	258.650	ml/mol	McGowan Method
tf	494.70	K	Sublimation thermodynamics of four fluoroquinolone antimicrobial compounds

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
psub	1.79e-06	kPa	431.15	Sublimation thermodynamics of four fluoroquinolone antimicrobial compounds
psub	2.13e-06	kPa	433.15	Sublimation thermodynamics of four fluoroquinolone antimicrobial compounds

psub	2.50e-06	kPa	435.15	Sublimation thermodynamics of four fluoroquinolone antimicrobial compounds
psub	2.92e-06	kPa	437.15	Sublimation thermodynamics of four fluoroquinolone antimicrobial compounds
psub	3.41e-06	kPa	439.15	Sublimation thermodynamics of four fluoroquinolone antimicrobial compounds
psub	4.04e-06	kPa	441.15	Sublimation thermodynamics of four fluoroquinolone antimicrobial compounds
psub	4.71e-06	kPa	443.15	Sublimation thermodynamics of four fluoroquinolone antimicrobial compounds
psub	5.49e-06	kPa	445.15	Sublimation thermodynamics of four fluoroquinolone antimicrobial compounds
psub	6.61e-06	kPa	447.15	Sublimation thermodynamics of four fluoroquinolone antimicrobial compounds
psub	7.56e-06	kPa	449.15	Sublimation thermodynamics of four fluoroquinolone antimicrobial compounds
psub	8.91e-06	kPa	451.15	Sublimation thermodynamics of four fluoroquinolone antimicrobial compounds
psub	1.03e-05	kPa	453.15	Sublimation thermodynamics of four fluoroquinolone antimicrobial compounds

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Sublimation thermodynamics of four fluoroquinolone antimicrobial compounds:	https://www.doi.org/10.1016/j.jct.2016.10.010
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
psub:	Sublimation pressure
tf:	Normal melting (fusion) point

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