2-(2-methyl-3-chloroanilino)nicotinic acid

Other names: 2-((3-chloro-2-methylphenyl)amino)nicotinic acid
clonixic acid
Inchi: InChI=1S/C13H11ClN2O2/c1-8-10(14)5-2-6-11(8)16-12-9(13(17)18)4-3-7-15-12/h2-7H,1
InchiKey: CLOMYZFHNHFSIQ-UHFFFAOYSA-N
Formula: C13H11ClN2O2
SMILES: Cc1c(Cl)cccc1Nc1ncccc1C(=O)O
Mol. weight [g/mol]: 262.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.26		Crippen Method
logp	3.485		Crippen Method
mcvol	186.150	ml/mol	McGowan Method
tf	505.75	K	A thermodynamic study of sublimation, dissolution and distribution processes of anti-inflammatory drug Clonixin

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
psub	7.53e-04	kPa	419.15	A thermodynamic study of sublimation, dissolution and distribution processes of anti-inflammatory drug Clonixin
psub	8.67e-04	kPa	421.15	A thermodynamic study of sublimation, dissolution and distribution processes of anti-inflammatory drug Clonixin

psub	9.66e-04	kPa	423.15	A thermodynamic study of sublimation, dissolution and distribution processes of anti-inflammatory drug Clonixin
psub	1.12e-03	kPa	425.15	A thermodynamic study of sublimation, dissolution and distribution processes of anti-inflammatory drug Clonixin
psub	1.29e-03	kPa	427.15	A thermodynamic study of sublimation, dissolution and distribution processes of anti-inflammatory drug Clonixin
psub	1.47e-03	kPa	429.15	A thermodynamic study of sublimation, dissolution and distribution processes of anti-inflammatory drug Clonixin
psub	1.69e-03	kPa	431.15	A thermodynamic study of sublimation, dissolution and distribution processes of anti-inflammatory drug Clonixin
psub	1.93e-03	kPa	433.15	A thermodynamic study of sublimation, dissolution and distribution processes of anti-inflammatory drug Clonixin
psub	2.21e-03	kPa	435.15	A thermodynamic study of sublimation, dissolution and distribution processes of anti-inflammatory drug Clonixin

psub	2.48e-03	kPa	437.15	A thermodynamic study of sublimation, dissolution and distribution processes of anti-inflammatory drug Clonixin
psub	2.88e-03	kPa	439.15	A thermodynamic study of sublimation, dissolution and distribution processes of anti-inflammatory drug Clonixin
psub	3.18e-03	kPa	441.15	A thermodynamic study of sublimation, dissolution and distribution processes of anti-inflammatory drug Clonixin
psub	3.74e-03	kPa	443.15	A thermodynamic study of sublimation, dissolution and distribution processes of anti-inflammatory drug Clonixin

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
A thermodynamic study of sublimation, dissolution and distribution processes of anti-inflammatory drug Clonixin:	https://www.doi.org/10.1016/j.jct.2019.01.006
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
psub:	Sublimation pressure
tf:	Normal melting (fusion) point