

Lonazolac, methylated

Inchi:	InChI=1S/C18H15ClN2O2/c1-23-16(22)11-15-17(12-7-9-14(19)10-8-12)21-18(20-15)13-5
InchiKey:	BHJIVYQLXBERAM-UHFFFAOYSA-N
Formula:	C18H15ClN2O2
SMILES:	<chem>COC(=O)CC1=NC(c2ccccc2)N=C1c1ccc(Cl)cc1</chem>
Mol. weight [g/mol]:	326.78

Physical Properties

Property code	Value	Unit	Source
gf	380.79	kJ/mol	Joback Method
hf	81.24	kJ/mol	Joback Method
hfus	42.93	kJ/mol	Joback Method
hvap	89.00	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.846		Crippen Method
mvol	237.140	ml/mol	McGowan Method
pc	2342.82	kPa	Joback Method
rinpol	2685.00		NIST Webbook
tb	914.26	K	Joback Method
tc	1183.00	K	Joback Method
tf	640.60	K	Joback Method
vc	0.911	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	725.52	J/mol×K	914.26	Joback Method
cpg	737.98	J/mol×K	959.05	Joback Method
cpg	748.37	J/mol×K	1003.84	Joback Method
cpg	756.73	J/mol×K	1048.63	Joback Method
cpg	763.08	J/mol×K	1093.42	Joback Method
cpg	767.45	J/mol×K	1138.21	Joback Method
cpg	769.87	J/mol×K	1183.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R201744&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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