

Ethyl loflazepate

Other names:	1H-1,4-Benzodiazepine-3-carboxylic acid, 7-chloro-5-(2-fluorophenyl)-2,3-dihydro-2-oxo-, ethyl ester CM 6912 Ethyl 7-chloro-5-(2-fluorophenyl)-2,3-dihydro-2-oxo-1H-1,4-benzodiazepine-3-carboxylate Ethyl fluclozepam Loflazepic acid, ethyl ester Victan Meilax
Inchi:	InChI=1S/C18H14ClFN2O3/c1-2-25-18(24)16-17(23)21-14-8-7-10(19)9-12(14)15(22-16)
InchiKey:	CUCHJCMWNFEYOM-UHFFFAOYSA-N
Formula:	C18H14ClFN2O3
SMILES:	CCOC(=O)C1N=C(c2ccccc2F)c2cc(Cl)ccc2NC1=O
Mol. weight [g/mol]:	360.77
CAS:	29177-84-2

Physical Properties

Property code	Value	Unit	Source
gf	-5.27	kJ/mol	Joback Method
hf	-354.98	kJ/mol	Joback Method
hfus	48.36	kJ/mol	Joback Method
hvap	93.35	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.200		Crippen Method
mcvol	244.780	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
tb	982.02	K	Joback Method
tc	1245.19	K	Joback Method
tf	754.66	K	Joback Method
vc	0.939	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	754.54	J/molxK	982.02	Joback Method
cpg	763.80	J/molxK	1025.88	Joback Method

cpg	770.87	J/mol×K	1069.74	Joback Method
cpg	775.71	J/mol×K	1113.61	Joback Method
cpg	778.30	J/mol×K	1157.47	Joback Method
cpg	778.61	J/mol×K	1201.33	Joback Method
cpg	776.60	J/mol×K	1245.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29177842&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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