

Milnacipran

Inchi:	InChI=1S/C15H22N2O/c1-3-17(4-2)14(18)15(10-13(15)11-16)12-8-6-5-7-9-12/h5-9,13H,
InchiKey:	GJJFMKBJSRMPLA-UHFFFAOYSA-N
Formula:	C15H22N2O
SMILES:	CCN(CC)C(=O)C1(c2ccccc2)CC1CN
Mol. weight [g/mol]:	246.35
CAS:	92623-85-3

Physical Properties

Property code	Value	Unit	Source
gf	283.69	kJ/mol	Joback Method
hf	-59.96	kJ/mol	Joback Method
hfus	31.37	kJ/mol	Joback Method
hvap	69.14	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	1.771		Crippen Method
mvol	209.120	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
rinpol	1952.00		NIST Webbook
tb	710.43	K	Joback Method
tc	933.82	K	Joback Method
tf	488.49	K	Joback Method
vc	0.774	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.84	J/molxK	710.43	Joback Method
cpg	627.16	J/molxK	747.66	Joback Method
cpg	643.63	J/molxK	784.89	Joback Method
cpg	659.42	J/molxK	822.12	Joback Method
cpg	674.73	J/molxK	859.36	Joback Method
cpg	689.74	J/molxK	896.59	Joback Method
cpg	704.64	J/molxK	933.82	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92623853&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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