O-Desmethyl-cis-tramadol

Inchi: InChI=1S/C15H23NO2/c1-16(2)11-13-6-3-4-9-15(13,18)12-7-5-8-14(17)10-12/h5,7-8,10,
InchiKey: UWJUQVWARXYRCG-UHFFFAOYSA-N
Formula: C15H23NO2
SMILES: CN(C)CC1CCCCC1(O)c1cccc(O)c1
Mol. weight [g/mol]: 249.35
CAS: 144830-14-8

Physical Properties

Property code	Value	Unit	Source
gf	18.42	kJ/mol	Joback Method
hf	-329.19	kJ/mol	Joback Method
hfus	28.15	kJ/mol	Joback Method
hvap	81.96	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.332		Crippen Method
mcvol	209.310	ml/mol	McGowan Method
pc	2856.62	kPa	Joback Method
rinpol	2074.20		NIST Webbook
rinpol	2074.20		NIST Webbook
tb	769.64	K	Joback Method
tc	992.11	K	Joback Method
tf	517.28	K	Joback Method
vc	0.701	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.61	J/mol×K	769.64	Joback Method
cpg	668.62	J/mol×K	806.72	Joback Method
cpg	685.08	J/mol×K	843.80	Joback Method
cpg	701.18	J/mol×K	880.88	Joback Method
cpg	717.13	J/mol×K	917.95	Joback Method
cpg	733.11	J/mol×K	955.03	Joback Method
cpg	749.35	J/mol×K	992.11	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C144830148&Units=SI

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