N-Desmethyltapentadol

Inchi: InChI=1S/C13H21NO/c1-4-13(10(2)9-14-3)11-6-5-7-12(15)8-11/h5-8,10,13-15H,4,9H2,1-
InchiKey: PQQINTFVECNXLC-UHFFFAOYSA-N
Formula: C13H21NO
SMILES: CCC(c1cccc(O)c1)C(C)CNC
Mol. weight [g/mol]: 207.31
CAS: 1246819-18-0

Physical Properties

Property code	Value	Unit	Source
gf	100.88	kJ/mol	Joback Method
hf	-209.52	kJ/mol	Joback Method
hfus	27.30	kJ/mol	Joback Method
hvap	65.48	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.741		Crippen Method
mcvol	186.120	ml/mol	McGowan Method
pc	2611.07	kPa	Joback Method
rinpol	1711.10		NIST Webbook
rinpol	1711.10		NIST Webbook
tb	653.43	K	Joback Method
tc	869.00	K	Joback Method
tf	397.07	K	Joback Method
vc	0.644	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.03	J/mol×K	653.43	Joback Method
cpg	525.06	J/mol×K	689.36	Joback Method
cpg	540.12	J/mol×K	725.29	Joback Method
cpg	554.27	J/mol×K	761.21	Joback Method
cpg	567.62	J/mol×K	797.14	Joback Method
cpg	580.23	J/mol×K	833.07	Joback Method
cpg	592.21	J/mol×K	869.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1246819180&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
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
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