Norapoatropine

Inchi: InChI=1S/C16H19NO2/c1-11(12-5-3-2-4-6-12)16(18)19-15-9-13-7-8-14(10-15)17-13/h2-
InchiKey: RDIVNYCOUBHXRH-UHFFFAOYSA-N
Formula: C16H19NO2
SMILES: C=C(C(=O)OC1CC2CCC(C1)N2)c1ccccc1
Mol. weight [g/mol]: 257.33
CAS: 78886-97-2

Physical Properties

Property code	Value	Unit	Source
gf	218.92	kJ/mol	Joback Method
hf	-115.45	kJ/mol	Joback Method
hfus	34.16	kJ/mol	Joback Method
hvap	68.67	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	2.526		Crippen Method
mcvol	203.940	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinpol	2160.80		NIST Webbook
rinpol	2160.80		NIST Webbook
tb	730.91	K	Joback Method
tc	975.44	K	Joback Method
tf	482.57	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.88	J/mol×K	730.91	Joback Method
cpg	623.99	J/mol×K	771.67	Joback Method
cpg	641.60	J/mol×K	812.42	Joback Method
cpg	657.79	J/mol×K	853.18	Joback Method
cpg	672.67	J/mol×K	893.93	Joback Method
cpg	686.33	J/mol×K	934.69	Joback Method
cpg	698.86	J/mol×K	975.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C78886972&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