Aponorscopolamine

Inchi: InChI=1S/C16H19NO4/c18-8-11(9-4-2-1-3-5-9)16(19)20-10-6-12-14-15(21-14)13(7-10)1
InchiKey: MOYZEMOPQDTDHA-ZOONQSOGSA-N
Formula: C16H19NO4
SMILES: O=C(OC1CC2NC(C1)C1OC21)C(CO)c1ccccc1
Mol. weight [g/mol]: 289.33

Physical Properties

Property code	Value	Unit	Source
gf	-8.51	kJ/mol	Joback Method
hf	-455.82	kJ/mol	Joback Method
hfus	48.70	kJ/mol	Joback Method
hvap	89.32	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	0.576		Crippen Method
mcvol	209.120	ml/mol	McGowan Method
pc	2665.27	kPa	Joback Method
rinpol	2056.00		NIST Webbook
tb	846.57	K	Joback Method
tc	1069.63	K	Joback Method
tf	591.42	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.09	J/mol×K	846.57	Joback Method
cpg	716.52	J/mol×K	883.75	Joback Method
cpg	730.04	J/mol×K	920.92	Joback Method
cpg	742.75	J/mol×K	958.10	Joback Method
cpg	754.78	J/mol×K	995.28	Joback Method
cpg	766.22	J/mol×K	1032.45	Joback Method
cpg	777.18	J/mol×K	1069.63	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=R512693&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