

Ephedrine, N-propyloxycarbonyl-

Other names:	Ephedrine, N-propoxycarbonyl
Inchi:	InChI=1S/C14H21NO3/c1-4-10-18-14(17)15(3)11(2)13(16)12-8-6-5-7-9-12/h5-9,11,13,16
InchiKey:	KZOUQPHJQWGH-UHFFFAOYSA-N
Formula:	C14H21NO3
SMILES:	CCCOC(=O)N(C)C(C)C(O)c1ccccc1
Mol. weight [g/mol]:	251.32

Physical Properties

Property code	Value	Unit	Source
gf	-85.43	kJ/mol	Joback Method
hf	-435.82	kJ/mol	Joback Method
hfus	28.91	kJ/mol	Joback Method
hvap	76.14	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.587		Crippen Method
mvol	207.650	ml/mol	McGowan Method
pc	2313.61	kPa	Joback Method
tb	726.43	K	Joback Method
tc	921.38	K	Joback Method
tf	409.41	K	Joback Method
vc	0.760	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.40	J/molxK	726.43	Joback Method
cpg	609.45	J/molxK	758.92	Joback Method
cpg	622.61	J/molxK	791.41	Joback Method
cpg	634.92	J/molxK	823.91	Joback Method
cpg	646.42	J/molxK	856.40	Joback Method
cpg	657.14	J/molxK	888.89	Joback Method
cpg	667.12	J/molxK	921.38	Joback Method

Sources

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=U314784&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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