Phentemine, N-propyloxycarbonyl-

Other names: Phentermine, N-propoxycarbonyl
Inchi: InChI=1S/C14H21NO2/c1-4-10-17-13(16)15-14(2,3)11-12-8-6-5-7-9-12/h5-9H,4,10-11H2
InchiKey: NUOIHVQVAOFTOB-UHFFFAOYSA-N
Formula: C14H21NO2
SMILES: CCCOC(=O)NC(C)(C)Cc1ccccc1
Mol. weight [g/mol]: 235.32

Physical Properties

Property code	Value	Unit	Source
gf	37.72	kJ/mol	Joback Method
hf	-295.84	kJ/mol	Joback Method
hfus	26.53	kJ/mol	Joback Method
hvap	63.33	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.144		Crippen Method
mcvol	201.780	ml/mol	McGowan Method
pc	2157.31	kPa	Joback Method
tb	669.63	K	Joback Method
tc	880.46	K	Joback Method
tf	401.20	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.38	J/mol×K	669.63	Joback Method
cpg	568.79	J/mol×K	704.77	Joback Method
cpg	584.11	J/mol×K	739.91	Joback Method
cpg	598.40	J/mol×K	775.05	Joback Method
cpg	611.72	J/mol×K	810.19	Joback Method
cpg	624.11	J/mol×K	845.32	Joback Method
cpg	635.62	J/mol×K	880.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U314783&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume