Propanamide, N-phenyl-N-4-piperidinyl-

Other names: Norfentanyl
N-phenyl-N-piperidin-4-ylpropionamide
Inchi: InChI=1S/C14H20N2O/c1-2-14(17)16(12-6-4-3-5-7-12)13-8-10-15-11-9-13/h3-7,13,15H,
InchiKey: PMCBDBWCQQBSRJ-UHFFFAOYSA-N
Formula: C14H20N2O
SMILES: CCC(=O)N(c1ccccc1)C1CCNCC1
Mol. weight [g/mol]: 232.32
CAS: 1609-66-1

Physical Properties

Property code	Value	Unit	Source
gf	273.43	kJ/mol	Joback Method
hf	-48.68	kJ/mol	Joback Method
hfus	32.10	kJ/mol	Joback Method
hvap	65.01	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.182		Crippen Method
mcvol	195.030	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
rinpol	2006.60		NIST Webbook
rinpol	2006.60		NIST Webbook
tb	680.81	K	Joback Method
tc	917.94	K	Joback Method
tf	468.77	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.17	J/mol×K	680.81	Joback Method
cpg	566.76	J/mol×K	720.33	Joback Method
cpg	584.85	J/mol×K	759.85	Joback Method
cpg	601.50	J/mol×K	799.37	Joback Method
cpg	616.79	J/mol×K	838.89	Joback Method

cpg	630.78	J/mol×K	878.41	Joback Method
cpg	643.54	J/mol×K	917.94	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=C1609661&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume