2-n-Pentyl-1,2,3,4-tetrahydroquinoline

Inchi: InChI=1S/C14H21N/c1-2-3-4-8-13-11-10-12-7-5-6-9-14(12)15-13/h5-7,9,13,15H,2-4,8,10
InchiKey: COWWTNSCQZQEAB-UHFFFAOYSA-N
Formula: C14H21N
SMILES: CCCCCC1CCc2ccccc2N1
Mol. weight [g/mol]: 203.32

Physical Properties

Property code	Value	Unit	Source
gf	306.14	kJ/mol	Joback Method
hf	-2.78	kJ/mol	Joback Method
hfus	31.29	kJ/mol	Joback Method
hvap	56.54	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.994		Crippen Method
mcvol	183.480	ml/mol	McGowan Method
pc	2342.82	kPa	Joback Method
rinpol	1765.00		NIST Webbook
rinpol	1765.00		NIST Webbook
tb	610.94	K	Joback Method
tc	831.33	K	Joback Method
tf	405.93	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.22	J/mol×K	610.94	Joback Method
cpg	499.55	J/mol×K	647.67	Joback Method
cpg	517.68	J/mol×K	684.40	Joback Method
cpg	534.68	J/mol×K	721.13	Joback Method
cpg	550.61	J/mol×K	757.87	Joback Method
cpg	565.52	J/mol×K	794.60	Joback Method
cpg	579.46	J/mol×K	831.33	Joback Method

Sources

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=R398279&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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