

Levopropacetoperane

Other names: 1-Phenyl-1-(2'-piperidyl)-1-acetoxymethane

Phacetoperane

RP-8228

Inchi: InChI=1S/C14H19NO2/c1-11(16)17-14(12-7-3-2-4-8-12)13-9-5-6-10-15-13/h2-4,7-8,13-1

InchiKey: BKPLVPRTTWIDNL-UHFFFAOYSA-N

Formula: C14H19NO2

SMILES: CC(=O)OC(c1ccccc1)C1CCCCN1

Mol. weight [g/mol]: 233.31

CAS: 24558-01-8

Physical Properties

Property code	Value	Unit	Source
gf	55.21	kJ/mol	Joback Method
hf	-253.71	kJ/mol	Joback Method
hfus	26.75	kJ/mol	Joback Method
hvap	64.99	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.433		Crippen Method
mcvol	190.920	ml/mol	McGowan Method
pc	2637.96	kPa	Joback Method
tb	690.35	K	Joback Method
tc	932.60	K	Joback Method
tf	443.53	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.99	J/molxK	690.35	Joback Method
cpg	555.28	J/molxK	730.72	Joback Method
cpg	573.06	J/molxK	771.10	Joback Method
cpg	589.39	J/molxK	811.47	Joback Method
cpg	604.30	J/molxK	851.85	Joback Method
cpg	617.83	J/molxK	892.22	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C24558018&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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