

LEVOPHACETOPERANE

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

Physical Properties

Property code	Value	Unit	Source
hf	-333.05	kJ/mol	Cheméo Relay (1.0)
hfus	26.75	kJ/mol	Joback Method
logp	2.433		Crippen Method
mcvol	190.920	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.99	J/mol×K	690.35	Joback Method
cpg	555.28	J/mol×K	730.72	Joback Method
cpg	573.06	J/mol×K	771.10	Joback Method
cpg	589.39	J/mol×K	811.47	Joback Method
cpg	604.30	J/mol×K	851.85	Joback Method
cpg	617.83	J/mol×K	892.22	Joback Method
cpg	630.00	J/mol×K	932.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C24558018&Units=SI>
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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