3-Phenylacetoxy-6,7-epoxynortropane

Inchi: InChI=1S/C15H17NO3/c17-13(6-9-4-2-1-3-5-9)18-10-7-11-14-15(19-14)12(8-10)16-11/h1
InchiKey: CTEVTHIFBCUTCT-NRBJTNBDSA-N
Formula: C15H17NO3
SMILES: O=C(Cc1ccccc1)OC1CC2NC(C1)C1OC21
Mol. weight [g/mol]: 259.30

Physical Properties

Property code	Value	Unit	Source
gf	122.33	kJ/mol	Joback Method
hf	-277.67	kJ/mol	Joback Method
hfus	45.55	kJ/mol	Joback Method
hvap	70.80	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	1.042		Crippen Method
mcvol	189.160	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
rinpol	1968.00		NIST Webbook
rinpol	1968.00		NIST Webbook
tb	731.95	K	Joback Method
tc	970.17	K	Joback Method
tf	534.33	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	588.13	J/mol×K	731.95	Joback Method
cpg	605.68	J/mol×K	771.65	Joback Method
cpg	621.95	J/mol×K	811.36	Joback Method
cpg	637.05	J/mol×K	851.06	Joback Method
cpg	651.11	J/mol×K	890.76	Joback Method
cpg	664.26	J/mol×K	930.47	Joback Method
cpg	676.62	J/mol×K	970.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R421631&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume