

2-Acetoxy-3-(2-cyclopentylphenoxy)propylamine,

Other names: N-acetyl-N-tert-butyl-4-(2-cyclopentylphenoxy)propylamine
Inchi: InChI=1S/C22H33NO4/c1-16(24)23(22(3,4)5)14-19(27-17(2)25)15-26-21-13-9-8-12-20(2)

InchiKey: PSAZFLWDPVWMY-UHFFFAOYSA-N
Formula: C22H33NO4
SMILES: CC(=O)OC(COc1cccc1C1CCCC1)CN(C(C)=O)C(C)(C)C
Mol. weight [g/mol]: 375.50

Physical Properties

Property code	Value	Unit	Source
gf	-82.97	kJ/mol	Joback Method
hf	-647.97	kJ/mol	Joback Method
hfus	37.98	kJ/mol	Joback Method
hvap	86.43	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.302		Crippen Method
mvol	311.080	ml/mol	McGowan Method
pc	1354.63	kPa	Joback Method
rinpol	2205.00		NIST Webbook
rinpol	2205.00		NIST Webbook
tb	911.05	K	Joback Method
tc	1132.46	K	Joback Method
tf	551.75	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1032.44	J/molxK	911.05	Joback Method
cpg	1049.48	J/molxK	947.95	Joback Method
cpg	1065.11	J/molxK	984.85	Joback Method
cpg	1079.40	J/molxK	1021.76	Joback Method
cpg	1092.44	J/molxK	1058.66	Joback Method
cpg	1104.31	J/molxK	1095.56	Joback Method
cpg	1115.09	J/molxK	1132.46	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=U280754&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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