N,N-dimethyl-3-[1-(phenylmethyl)cycloheptyl]oxy

Inchi: InChI=1S/C19H31NO/c1-20(2)15-10-16-21-19(13-8-3-4-9-14-19)17-18-11-6-5-7-12-18/h5
InchiKey: FYJJXENSONZJRG-UHFFFAOYSA-N
Formula: C19H31NO
SMILES: CN(C)CCCOC1(Cc2ccccc2)CCCCCC1
Mol. weight [g/mol]: 289.46

Physical Properties

Property code	Value	Unit	Source
gf	234.15	kJ/mol	Joback Method
hf	-200.25	kJ/mol	Joback Method
hfus	26.65	kJ/mol	Joback Method
hvap	64.07	kJ/mol	Joback Method
log10ws	-1.62		Aqueous Solubility Prediction Method
logp	4.290		Crippen Method
mcvol	259.800	ml/mol	McGowan Method
pc	1659.19	kPa	Joback Method
tb	719.72	K	Joback Method
tc	939.64	K	Joback Method
tf	412.77	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.41	J/mol×K	719.72	Joback Method
cpg	801.77	J/mol×K	756.37	Joback Method
cpg	823.85	J/mol×K	793.03	Joback Method
cpg	844.81	J/mol×K	829.68	Joback Method
cpg	864.79	J/mol×K	866.33	Joback Method
cpg	883.94	J/mol×K	902.98	Joback Method
cpg	902.42	J/mol×K	939.64	Joback Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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