trans-2-Phenylcyclopropylamine, heptafluorobutyryl

Other names: Tranylcypromine, HFB

Inchi: InChI=1S/C13H10F7NO/c14-11(15,12(16,17)13(18,19)20)10(22)21-9-6-8(9)7-4-2-1-3-5-7

InchiKey: SGOGAADMNOIARZ-DTWKUNHWSA-N

Formula: C13H10F7NO

SMILES: O=C(NC1CC1c1ccccc1)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 329.21

Physical Properties

Property code	Value	Unit	Source
gf	-1170.65	kJ/mol	Joback Method
hf	-1480.79	kJ/mol	Joback Method
hfus	28.69	kJ/mol	Joback Method
hvap	49.99	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.492		Crippen Method
mcvol	183.350	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
tb	614.83	K	Joback Method
tc	803.65	K	Joback Method
tf	390.37	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.74	J/mol×K	614.83	Joback Method
cpg	537.69	J/mol×K	646.30	Joback Method
cpg	550.50	J/mol×K	677.77	Joback Method
cpg	562.26	J/mol×K	709.24	Joback Method
cpg	573.06	J/mol×K	740.71	Joback Method
cpg	583.00	J/mol×K	772.18	Joback Method
cpg	592.16	J/mol×K	803.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U90230&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

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