Cyclohexanecarboxylic acid, pentafluorophenyl ester

Inchi: InChI=1S/C13H11F5O2/c14-7-8(15)10(17)12(11(18)9(7)16)20-13(19)6-4-2-1-3-5-6/h6H,1

InchiKey: YTMNGMCPLMPVPK-UHFFFAOYSA-N

Formula: C13H11F5O2

SMILES: O=C(Oc1c(F)c(F)c(F)c(F)c1F)C1CCCCC1

Mol. weight [g/mol]: 294.22

Physical Properties

Property code	Value	Unit	Source
gf	-1060.68	kJ/mol	Joback Method
hf	-1303.50	kJ/mol	Joback Method
hfus	31.54	kJ/mol	Joback Method
hvap	55.62	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	3.868		Crippen Method
mcvol	175.700	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
rinpol	1487.00		NIST Webbook
tb	640.61	K	Joback Method
tc	835.72	K	Joback Method
tf	407.78	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.86	J/mol×K	640.61	Joback Method
cpg	485.96	J/mol×K	673.13	Joback Method
cpg	499.27	J/mol×K	705.65	Joback Method
cpg	511.79	J/mol×K	738.16	Joback Method
cpg	523.52	J/mol×K	770.68	Joback Method
cpg	534.47	J/mol×K	803.20	Joback Method
cpg	544.64	J/mol×K	835.72	Joback Method

Sources

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=U354648&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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