3-Cyclopentylpropionic acid, pentafluorophenyl ester

Inchi: InChI=1S/C14H13F5O2/c15-9-10(16)12(18)14(13(19)11(9)17)21-8(20)6-5-7-3-1-2-4-7/h7

InchiKey: UOWZPDYHJCKUMA-UHFFFAOYSA-N

Formula: C14H13F5O2

SMILES: O=C(CCC1CCCC1)Oc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 308.24

Physical Properties

Property code	Value	Unit	Source
gf	-1040.16	kJ/mol	Joback Method
hf	-1317.98	kJ/mol	Joback Method
hfus	36.23	kJ/mol	Joback Method
hvap	57.67	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.258		Crippen Method
mcvol	189.790	ml/mol	McGowan Method
pc	1882.17	kPa	Joback Method
rinpol	1578.00		NIST Webbook
tb	659.22	K	Joback Method
tc	847.07	K	Joback Method
tf	422.57	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.37	J/mol×K	659.22	Joback Method
cpg	535.33	J/mol×K	690.53	Joback Method
cpg	548.52	J/mol×K	721.84	Joback Method
cpg	560.97	J/mol×K	753.15	Joback Method
cpg	572.67	J/mol×K	784.45	Joback Method
cpg	583.65	J/mol×K	815.76	Joback Method
cpg	593.90	J/mol×K	847.07	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=U354329&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