3-Cyclopentylpropionic acid, 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C13H16F8O2/c14-10(15)12(18,19)13(20,21)11(16,17)7-23-9(22)6-5-8-3-1-2-4-

InchiKey: KQTPXIPKMKKEMP-UHFFFAOYSA-N

Formula: C13H16F8O2

SMILES: O=C(CCC1CCCC1)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 356.25

Physical Properties

Property code	Value	Unit	Source
gf	-1691.19	kJ/mol	Joback Method
hf	-2096.38	kJ/mol	Joback Method
hfus	25.02	kJ/mol	Joback Method
hvap	43.13	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.671		Crippen Method
mcvol	204.770	ml/mol	McGowan Method
pc	1556.12	kPa	Joback Method
rinpol	1395.00		NIST Webbook
tb	572.44	K	Joback Method
tc	734.50	K	Joback Method
tf	316.31	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.85	J/mol×K	572.44	Joback Method
cpg	593.73	J/mol×K	599.45	Joback Method
cpg	608.67	J/mol×K	626.46	Joback Method
cpg	622.70	J/mol×K	653.47	Joback Method
cpg	635.87	J/mol×K	680.48	Joback Method
cpg	648.23	J/mol×K	707.49	Joback Method
cpg	659.82	J/mol×K	734.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354326&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume