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

Inchi: InChI=1S/C12H14F8O2/c13-9(14)11(17,18)12(19,20)10(15,16)6-22-8(21)7-4-2-1-3-5-7/h

InchiKey: RXDNUAJMLDMDNI-UHFFFAOYSA-N

Formula: C12H14F8O2

SMILES: O=C(OCC(F)(F)C(F)(F)C(F)(F)C(F)F)C1CCCCC1

Mol. weight [g/mol]: 342.23

Physical Properties

Property code	Value	Unit	Source
gf	-1711.71	kJ/mol	Joback Method
hf	-2081.90	kJ/mol	Joback Method
hfus	20.33	kJ/mol	Joback Method
hvap	41.08	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	4.281		Crippen Method
mcvol	190.680	ml/mol	McGowan Method
pc	1716.03	kPa	Joback Method
rinpol	1273.00		NIST Webbook
tb	553.83	K	Joback Method
tc	721.29	K	Joback Method
tf	301.52	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.01	J/mol×K	553.83	Joback Method
cpg	544.25	J/mol×K	581.74	Joback Method
cpg	559.49	J/mol×K	609.65	Joback Method
cpg	573.78	J/mol×K	637.56	Joback Method
cpg	587.15	J/mol×K	665.47	Joback Method
cpg	599.66	J/mol×K	693.38	Joback Method
cpg	611.35	J/mol×K	721.29	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=U354645&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