1,2-Cyclohexanedicarboxylic acid, 2-fluorophenyl propyl ester

Inchi: InChI=1S/C17H21FO4/c1-2-11-21-16(19)12-7-3-4-8-13(12)17(20)22-15-10-6-5-9-14(15)1

InchiKey: QKUHCCQYWXSVIK-UHFFFAOYSA-N

Formula: C17H21FO4

SMILES: CCCOC(=O)C1CCCCC1C(=O)Oc1ccccc1F

Mol. weight [g/mol]: 308.34

Physical Properties

Property code	Value	Unit	Source
gf	-450.87	kJ/mol	Joback Method
hf	-820.88	kJ/mol	Joback Method
hfus	35.00	kJ/mol	Joback Method
hvap	73.99	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.491		Crippen Method
mcvol	232.420	ml/mol	McGowan Method
pc	1865.94	kPa	Joback Method
rinpol	2116.00		NIST Webbook
rinpol	2116.00		NIST Webbook
tb	786.75	K	Joback Method
tc	1004.90	K	Joback Method
tf	468.34	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.58	J/mol×K	786.75	Joback Method
cpg	726.37	J/mol×K	823.11	Joback Method
cpg	741.79	J/mol×K	859.47	Joback Method
cpg	755.83	J/mol×K	895.83	Joback Method
cpg	768.53	J/mol×K	932.18	Joback Method
cpg	779.89	J/mol×K	968.54	Joback Method
cpg	789.93	J/mol×K	1004.90	Joback Method

Sources

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=U339779&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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