1,2-Cyclohexanedicarboxylic acid, 3-fluorophenyl isobutyl ester

Inchi: InChI=1S/C18H23FO4/c1-12(2)11-22-17(20)15-8-3-4-9-16(15)18(21)23-14-7-5-6-13(19)1

InchiKey: CJXSFEYBDVHQPW-UHFFFAOYSA-N

Formula: C18H23FO4

SMILES: CC(C)COC(=O)C1CCCCC1C(=O)Oc1cccc(F)c1

Mol. weight [g/mol]: 322.37

Physical Properties

Property code	Value	Unit	Source
gf	-444.89	kJ/mol	Joback Method
hf	-846.80	kJ/mol	Joback Method
hfus	34.06	kJ/mol	Joback Method
hvap	75.83	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	3.737		Crippen Method
mcvol	246.510	ml/mol	McGowan Method
pc	1731.78	kPa	Joback Method
rinpol	2154.00		NIST Webbook
tb	809.19	K	Joback Method
tc	1028.13	K	Joback Method
tf	464.61	K	Joback Method
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.51	J/mol×K	809.19	Joback Method
cpg	784.56	J/mol×K	845.68	Joback Method
cpg	800.15	J/mol×K	882.17	Joback Method
cpg	814.31	J/mol×K	918.66	Joback Method
cpg	827.05	J/mol×K	955.15	Joback Method
cpg	838.38	J/mol×K	991.64	Joback Method
cpg	848.33	J/mol×K	1028.13	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=U339399&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