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

Inchi: InChI=1S/C23H33FO4/c1-2-3-4-5-6-7-10-16-27-22(25)20-14-8-9-15-21(20)23(26)28-19-1

InchiKey: KKDVPZNHXGNWEO-UHFFFAOYSA-N

Formula: C23H33FO4

SMILES: CCCCCCCCCOC(=O)C1CCCCC1C(=O)Oc1cccc(F)c1

Mol. weight [g/mol]: 392.50

Physical Properties

Property code	Value	Unit	Source
gf	-400.35	kJ/mol	Joback Method
hf	-944.72	kJ/mol	Joback Method
hfus	50.54	kJ/mol	Joback Method
hvap	87.34	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	5.831		Crippen Method
mcvol	316.960	ml/mol	McGowan Method
pc	1196.48	kPa	Joback Method
rinpol	2706.00		NIST Webbook
rinpol	2706.00		NIST Webbook
tb	924.03	K	Joback Method
tc	1138.24	K	Joback Method
tf	535.96	K	Joback Method
vc	1.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1064.68	J/mol×K	924.03	Joback Method
cpg	1081.33	J/mol×K	959.73	Joback Method
cpg	1096.38	J/mol×K	995.43	Joback Method
cpg	1109.89	J/mol×K	1031.13	Joback Method
cpg	1121.88	J/mol×K	1066.83	Joback Method
cpg	1132.39	J/mol×K	1102.54	Joback Method
cpg	1141.44	J/mol×K	1138.24	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339403&Units=SI

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