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

Inchi: InChI=1S/C16H19FO4/c1-2-20-15(18)11-7-3-4-8-12(11)16(19)21-14-10-6-5-9-13(14)17/h

InchiKey: ZWTDJXITALZSQN-UHFFFAOYSA-N

Formula: C16H19FO4

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

Mol. weight [g/mol]: 294.32

Physical Properties

Property code	Value	Unit	Source
gf	-459.29	kJ/mol	Joback Method
hf	-800.24	kJ/mol	Joback Method
hfus	32.41	kJ/mol	Joback Method
hvap	71.76	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.101		Crippen Method
mcvol	218.330	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	2017.00		NIST Webbook
rinpol	2017.00		NIST Webbook
tb	763.87	K	Joback Method
tc	984.88	K	Joback Method
tf	457.07	K	Joback Method
vc	0.822	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.08	J/mol×K	763.87	Joback Method
cpg	669.80	J/mol×K	800.70	Joback Method
cpg	685.17	J/mol×K	837.54	Joback Method
cpg	699.19	J/mol×K	874.37	Joback Method
cpg	711.88	J/mol×K	911.21	Joback Method
cpg	723.25	J/mol×K	948.04	Joback Method
cpg	733.31	J/mol×K	984.88	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=U339778&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