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

Inchi: InChI=1S/C21H29FO4/c1-2-3-4-5-10-15-25-20(23)16-11-6-7-12-17(16)21(24)26-19-14-9

InchiKey: QIUIWYFKVQTRBT-UHFFFAOYSA-N

Formula: C21H29FO4

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

Mol. weight [g/mol]: 364.45

Physical Properties

Property code	Value	Unit	Source
gf	-417.19	kJ/mol	Joback Method
hf	-903.44	kJ/mol	Joback Method
hfus	45.36	kJ/mol	Joback Method
hvap	82.89	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	5.051		Crippen Method
mcvol	288.780	ml/mol	McGowan Method
pc	1372.76	kPa	Joback Method
rinpol	2513.00		NIST Webbook
rinpol	2513.00		NIST Webbook
tb	878.27	K	Joback Method
tc	1090.97	K	Joback Method
tf	513.42	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	943.73	J/mol×K	878.27	Joback Method
cpg	960.47	J/mol×K	913.72	Joback Method
cpg	975.71	J/mol×K	949.17	Joback Method
cpg	989.49	J/mol×K	984.62	Joback Method
cpg	1001.82	J/mol×K	1020.07	Joback Method
cpg	1012.74	J/mol×K	1055.52	Joback Method
cpg	1022.27	J/mol×K	1090.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339785&Units=SI
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

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