

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

Inchi:	InChI=1S/C19H25FO4/c1-2-3-6-12-23-18(21)16-10-4-5-11-17(16)19(22)24-15-9-7-8-14(2)
InchiKey:	WGKOKCUYGXKFSS-UHFFFAOYSA-N
Formula:	C19H25FO4
SMILES:	CCCCCOC(=O)C1CCCCC1C(=O)Oc1cccc(F)c1
Mol. weight [g/mol]:	336.40

Physical Properties

Property code	Value	Unit	Source
gf	-434.03	kJ/mol	Joback Method
hf	-862.16	kJ/mol	Joback Method
hfus	40.18	kJ/mol	Joback Method
hvap	78.44	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.271		Crippen Method
mvol	260.600	ml/mol	McGowan Method
pc	1591.08	kPa	Joback Method
rinpol	2293.00		NIST Webbook
rinpol	2293.00		NIST Webbook
tb	832.51	K	Joback Method
tc	1046.65	K	Joback Method
tf	490.88	K	Joback Method
vc	0.990	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.18	J/mol×K	832.51	Joback Method
cpg	841.99	J/mol×K	868.20	Joback Method
cpg	857.37	J/mol×K	903.89	Joback Method
cpg	871.34	J/mol×K	939.58	Joback Method
cpg	883.92	J/mol×K	975.27	Joback Method
cpg	895.13	J/mol×K	1010.96	Joback Method
cpg	904.99	J/mol×K	1046.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339400&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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