Isophthalic acid, 3,5-difluorophenyl hexyl ester

Inchi: InChI=1S/C20H20F2O4/c1-2-3-4-5-9-25-19(23)14-7-6-8-15(10-14)20(24)26-18-12-16(21

InchiKey: URAPRRYAWXICIE-UHFFFAOYSA-N

Formula: C20H20F2O4

SMILES: CCCCCCOC(=O)c1cccc(C(=O)Oc2cc(F)cc(F)c2)c1

Mol. weight [g/mol]: 362.37

Physical Properties

Property code	Value	Unit	Source
gf	-544.01	kJ/mol	Joback Method
hf	-899.30	kJ/mol	Joback Method
hfus	46.20	kJ/mol	Joback Method
hvap	83.33	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	4.921		Crippen Method
mcvol	263.560	ml/mol	McGowan Method
pc	1575.95	kPa	Joback Method
rinpol	2567.00		NIST Webbook
rinpol	2567.00		NIST Webbook
tb	876.42	K	Joback Method
tc	1090.09	K	Joback Method
tf	551.06	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.82	J/mol×K	876.42	Joback Method
cpg	806.87	J/mol×K	912.03	Joback Method
cpg	818.76	J/mol×K	947.64	Joback Method
cpg	829.50	J/mol×K	983.25	Joback Method
cpg	839.11	J/mol×K	1018.86	Joback Method
cpg	847.62	J/mol×K	1054.47	Joback Method
cpg	855.05	J/mol×K	1090.09	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=U344373&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

Latest version available from:
https://www.chemeo.com/cid/114-701-6/Isophthalic-acid-3-5-difluorophenyl-hexyl-ester.pdf
Generated by Cheméo on 2024-05-10 19:09:32.369240437 +0000 UTC m=+17657421.289817749.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.