Terephthalic acid, hexyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C20H19F3O4/c1-2-3-4-5-12-26-19(24)13-6-8-14(9-7-13)20(25)27-16-11-10-15

InchiKey: UULWOBHUSDCKOU-UHFFFAOYSA-N

Formula: C20H19F3O4

SMILES: CCCCCCOC(=O)c1ccc(C(=O)Oc2ccc(F)c(F)c2F)cc1

Mol. weight [g/mol]: 380.36

Physical Properties

Property code	Value	Unit	Source
gf	-748.45	kJ/mol	Joback Method
hf	-1106.88	kJ/mol	Joback Method
hfus	48.90	kJ/mol	Joback Method
hvap	83.17	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	5.060		Crippen Method
mcvol	265.330	ml/mol	McGowan Method
pc	1503.48	kPa	Joback Method
rinpol	2720.00		NIST Webbook
rinpol	2720.00		NIST Webbook
tb	880.67	K	Joback Method
tc	1090.49	K	Joback Method
tf	564.17	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.91	J/mol×K	880.67	Joback Method
cpg	812.49	J/mol×K	915.64	Joback Method
cpg	823.93	J/mol×K	950.61	Joback Method
cpg	834.25	J/mol×K	985.58	Joback Method
cpg	843.47	J/mol×K	1020.55	Joback Method
cpg	851.62	J/mol×K	1055.52	Joback Method
cpg	858.70	J/mol×K	1090.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415802&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