Terephthalic acid, nonyl 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C20H27F3O4/c1-3-4-5-6-7-8-9-14-26-18(24)16-10-12-17(13-11-16)19(25)27-1
InchiKey: LXRWIVQFRJPGTO-UHFFFAOYSA-N
Formula: C20H27F3O4
SMILES: CCCCCCCCCOC(=O)c1ccc(C(=O)OC(C)C(F)(F)F)cc1
Mol. weight [g/mol]: 388.42

Physical Properties

Property code	Value	Unit	Source
gf	-831.57	kJ/mol	Joback Method
hf	-1323.03	kJ/mol	Joback Method
hfus	45.08	kJ/mol	Joback Method
hvap	77.23	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	5.702		Crippen Method
mcvol	289.090	ml/mol	McGowan Method
pc	1241.58	kPa	Joback Method
rinpol	2439.00		NIST Webbook
rinpol	2439.00		NIST Webbook
tb	835.38	K	Joback Method
tc	1029.97	K	Joback Method
tf	487.61	K	Joback Method
vc	1.133	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	901.44	J/mol×K	835.38	Joback Method
cpg	916.60	J/mol×K	867.81	Joback Method
cpg	930.70	J/mol×K	900.24	Joback Method
cpg	943.78	J/mol×K	932.67	Joback Method
cpg	955.88	J/mol×K	965.10	Joback Method
cpg	967.03	J/mol×K	997.53	Joback Method
cpg	977.27	J/mol×K	1029.97	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415768&Units=SI

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