Phthalic acid, isobutyl 4-trifluoromethoxybenzyl ester

Inchi: InChI=1S/C20H19F3O5/c1-13(2)11-26-18(24)16-5-3-4-6-17(16)19(25)27-12-14-7-9-15(1

InchiKey: XMPGFYPGGRSAEO-UHFFFAOYSA-N

Formula: C20H19F3O5

SMILES: CC(C)COC(=O)c1ccccc1C(=O)OCc1ccc(OC(F)(F)F)cc1

Mol. weight [g/mol]: 396.36

Physical Properties

Property code	Value	Unit	Source
gf	-833.79	kJ/mol	Joback Method
hf	-1230.19	kJ/mol	Joback Method
hfus	39.92	kJ/mol	Joback Method
hvap	82.58	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	4.755		Crippen Method
mcvol	271.200	ml/mol	McGowan Method
pc	1551.22	kPa	Joback Method
rinpol	2245.00		NIST Webbook
rinpol	2245.00		NIST Webbook
tb	889.46	K	Joback Method
tc	1105.60	K	Joback Method
tf	548.78	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	830.74	J/mol×K	889.46	Joback Method
cpg	843.09	J/mol×K	925.48	Joback Method
cpg	854.21	J/mol×K	961.51	Joback Method
cpg	864.13	J/mol×K	997.53	Joback Method
cpg	872.90	J/mol×K	1033.55	Joback Method
cpg	880.55	J/mol×K	1069.57	Joback Method
cpg	887.11	J/mol×K	1105.60	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=U377685&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