Phthalic acid, isobutyl 2,2,2-trifluoro-1-phenylethyl ester

Inchi: InChI=1S/C20H19F3O4/c1-13(2)12-26-18(24)15-10-6-7-11-16(15)19(25)27-17(20(21,22)

InchiKey: NULJIZNCIIFYQB-UHFFFAOYSA-N

Formula: C20H19F3O4

SMILES: CC(C)COC(=O)c1ccccc1C(=O)OC(c1ccccc1)C(F)(F)F

Mol. weight [g/mol]: 380.36

Physical Properties

Property code	Value	Unit	Source
gf	-721.60	kJ/mol	Joback Method
hf	-1091.78	kJ/mol	Joback Method
hfus	35.60	kJ/mol	Joback Method
hvap	79.12	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	4.960		Crippen Method
mcvol	265.330	ml/mol	McGowan Method
pc	1601.28	kPa	Joback Method
rinpol	2134.00		NIST Webbook
rinpol	2134.00		NIST Webbook
tb	861.62	K	Joback Method
tc	1079.42	K	Joback Method
tf	499.03	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	805.75	J/mol×K	861.62	Joback Method
cpg	818.95	J/mol×K	897.92	Joback Method
cpg	830.95	J/mol×K	934.22	Joback Method
cpg	841.82	J/mol×K	970.52	Joback Method
cpg	851.61	J/mol×K	1006.82	Joback Method
cpg	860.39	J/mol×K	1043.12	Joback Method
cpg	868.22	J/mol×K	1079.42	Joback Method

Sources

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=U377701&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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