Terephthalic acid, butyl 2,2,2-trifluoro-1-phenylethyl ester

Inchi: InChI=1S/C20H19F3O4/c1-2-3-13-26-18(24)15-9-11-16(12-10-15)19(25)27-17(20(21,22)

InchiKey: UHNIWRFVWNGEMX-UHFFFAOYSA-N

Formula: C20H19F3O4

SMILES: CCCCOC(=O)c1ccc(C(=O)OC(c2ccccc2)C(F)(F)F)cc1

Mol. weight [g/mol]: 380.36

Physical Properties

Property code	Value	Unit	Source
gf	-719.16	kJ/mol	Joback Method
hf	-1086.50	kJ/mol	Joback Method
hfus	39.13	kJ/mol	Joback Method
hvap	79.50	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	5.104		Crippen Method
mcvol	265.330	ml/mol	McGowan Method
pc	1591.08	kPa	Joback Method
rinpol	2412.00		NIST Webbook
rinpol	2412.00		NIST Webbook
tb	862.06	K	Joback Method
tc	1077.35	K	Joback Method
tf	514.03	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	805.20	J/mol×K	862.06	Joback Method
cpg	818.27	J/mol×K	897.94	Joback Method
cpg	830.18	J/mol×K	933.82	Joback Method
cpg	840.99	J/mol×K	969.71	Joback Method
cpg	850.77	J/mol×K	1005.59	Joback Method
cpg	859.56	J/mol×K	1041.47	Joback Method
cpg	867.44	J/mol×K	1077.35	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=U415985&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