Terephthalic acid, butyl 4-trifluoromethoxybenzyl ester

Inchi: InChI=1S/C20H19F3O5/c1-2-3-12-26-18(24)15-6-8-16(9-7-15)19(25)27-13-14-4-10-17(1

InchiKey: GCJVKCAERDMRLW-UHFFFAOYSA-N

Formula: C20H19F3O5

SMILES: CCCCOC(=O)c1ccc(C(=O)OCc2ccc(OC(F)(F)F)cc2)cc1

Mol. weight [g/mol]: 396.36

Physical Properties

Property code	Value	Unit	Source
gf	-831.35	kJ/mol	Joback Method
hf	-1224.91	kJ/mol	Joback Method
hfus	43.45	kJ/mol	Joback Method
hvap	82.97	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	4.899		Crippen Method
mcvol	271.200	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
rinpol	2571.00		NIST Webbook
rinpol	2571.00		NIST Webbook
tb	889.90	K	Joback Method
tc	1103.99	K	Joback Method
tf	563.78	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	830.20	J/mol×K	889.90	Joback Method
cpg	842.46	J/mol×K	925.58	Joback Method
cpg	853.53	J/mol×K	961.26	Joback Method
cpg	863.44	J/mol×K	996.95	Joback Method
cpg	872.22	J/mol×K	1032.63	Joback Method
cpg	879.92	J/mol×K	1068.31	Joback Method
cpg	886.56	J/mol×K	1103.99	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=U415976&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