Terephthalic acid, butyl 4-(trifluoromethyl)benzyl ester

Inchi: InChI=1S/C20H19F3O4/c1-2-3-12-26-18(24)15-6-8-16(9-7-15)19(25)27-13-14-4-10-17(1

InchiKey: DALSFLCIPYNXOG-UHFFFAOYSA-N

Formula: C20H19F3O4

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

Mol. weight [g/mol]: 380.36

Physical Properties

Property code	Value	Unit	Source
gf	-726.35	kJ/mol	Joback Method
hf	-1092.69	kJ/mol	Joback Method
hfus	42.26	kJ/mol	Joback Method
hvap	80.56	kJ/mol	Joback Method
log10ws	-6.43		Crippen Method
logp	5.019		Crippen Method
mcvol	265.330	ml/mol	McGowan Method
pc	1562.28	kPa	Joback Method
rinpol	2816.00		NIST Webbook
rinpol	2816.00		NIST Webbook
tb	867.48	K	Joback Method
tc	1081.23	K	Joback Method
tf	541.55	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.43	J/mol×K	867.48	Joback Method
cpg	816.29	J/mol×K	903.10	Joback Method
cpg	828.02	J/mol×K	938.73	Joback Method
cpg	838.69	J/mol×K	974.35	Joback Method
cpg	848.34	J/mol×K	1009.98	Joback Method
cpg	857.02	J/mol×K	1045.60	Joback Method
cpg	864.78	J/mol×K	1081.23	Joback Method

Sources

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=U383031&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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