Terephthalic acid, 2-fluoro-6-(trifluoromethyl)benzyl isobutyl ester

Inchi: InChI=1S/C20H18F4O4/c1-12(2)10-27-18(25)13-6-8-14(9-7-13)19(26)28-11-15-16(20(22
InchiKey: AYOMEMHRFOATOW-UHFFFAOYSA-N
Formula: C20H18F4O4
SMILES: CC(C)COC(=O)c1ccc(C(=O)OCc2c(F)cccc2C(F)(F)F)cc1
Mol. weight [g/mol]: 398.35

Physical Properties

Property code	Value	Unit	Source
gf	-933.23	kJ/mol	Joback Method
hf	-1305.55	kJ/mol	Joback Method
hfus	41.43	kJ/mol	Joback Method
hvap	80.01	kJ/mol	Joback Method
log10ws	-6.52		Crippen Method
logp	5.014		Crippen Method
mcvol	267.100	ml/mol	McGowan Method
pc	1499.99	kPa	Joback Method
rinpol	2767.00		NIST Webbook
rinpol	2767.00		NIST Webbook
tb	871.29	K	Joback Method
tc	1082.89	K	Joback Method
tf	539.66	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	810.08	J/mol×K	871.29	Joback Method
cpg	822.54	J/mol×K	906.56	Joback Method
cpg	833.89	J/mol×K	941.82	Joback Method
cpg	844.17	J/mol×K	977.09	Joback Method
cpg	853.43	J/mol×K	1012.36	Joback Method
cpg	861.72	J/mol×K	1047.62	Joback Method
cpg	869.07	J/mol×K	1082.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382944&Units=SI
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

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