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

Inchi: InChI=1S/C24H14F8O4/c25-19-5-1-3-17(23(27,28)29)15(19)11-35-21(33)13-7-9-14(10-8

InchiKey: PZPUQQXKRSWMRW-UHFFFAOYSA-N

Formula: C24H14F8O4

SMILES: O=C(OCc1c(F)cccc1C(F)(F)F)c1ccc(C(=O)OCc2c(F)cccc2C(F)(F)F)cc1

Mol. weight [g/mol]: 518.35

Physical Properties

Property code	Value	Unit	Source
gf	-1580.36	kJ/mol	Joback Method
hf	-1962.43	kJ/mol	Joback Method
hfus	53.48	kJ/mol	Joback Method
hvap	88.34	kJ/mol	Joback Method
log10ws	-9.05		Crippen Method
logp	6.716		Crippen Method
mcvol	306.780	ml/mol	McGowan Method
pc	1245.09	kPa	Joback Method
rinpol	3226.00		NIST Webbook
rinpol	3226.00		NIST Webbook
tb	993.74	K	Joback Method
tc	1218.60	K	Joback Method
tf	655.98	K	Joback Method
vc	1.226	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	959.60	J/mol×K	993.74	Joback Method
cpg	969.14	J/mol×K	1031.22	Joback Method
cpg	977.64	J/mol×K	1068.69	Joback Method
cpg	985.20	J/mol×K	1106.17	Joback Method
cpg	991.92	J/mol×K	1143.65	Joback Method
cpg	997.88	J/mol×K	1181.13	Joback Method
cpg	1003.17	J/mol×K	1218.60	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=U382953&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