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

Inchi: InChI=1S/C24H26F4O4/c1-2-3-4-5-6-7-15-31-22(29)17-11-13-18(14-12-17)23(30)32-16-

InchiKey: RXYBBTSEQOZSGS-UHFFFAOYSA-N

Formula: C24H26F4O4

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

Mol. weight [g/mol]: 454.45

Physical Properties

Property code	Value	Unit	Source
gf	-897.11	kJ/mol	Joback Method
hf	-1382.83	kJ/mol	Joback Method
hfus	55.31	kJ/mol	Joback Method
hvap	89.30	kJ/mol	Joback Method
log10ws	-8.43		Crippen Method
logp	6.719		Crippen Method
mcvol	323.460	ml/mol	McGowan Method
pc	1130.62	kPa	Joback Method
rinpol	3209.00		NIST Webbook
rinpol	3209.00		NIST Webbook
tb	963.25	K	Joback Method
tc	1180.39	K	Joback Method
tf	599.74	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1042.70	J/mol×K	963.25	Joback Method
cpg	1055.93	J/mol×K	999.44	Joback Method
cpg	1067.94	J/mol×K	1035.63	Joback Method
cpg	1078.78	J/mol×K	1071.82	Joback Method
cpg	1088.51	J/mol×K	1108.01	Joback Method
cpg	1097.19	J/mol×K	1144.20	Joback Method
cpg	1104.90	J/mol×K	1180.39	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=U382949&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