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

Inchi: InChI=1S/C23H24F4O4/c1-2-3-4-5-6-14-30-21(28)16-10-12-17(13-11-16)22(29)31-15-18

InchiKey: LTDXBVRYXONSAP-UHFFFAOYSA-N

Formula: C23H24F4O4

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

Mol. weight [g/mol]: 440.43

Physical Properties

Property code	Value	Unit	Source
gf	-905.53	kJ/mol	Joback Method
hf	-1362.19	kJ/mol	Joback Method
hfus	52.72	kJ/mol	Joback Method
hvap	87.08	kJ/mol	Joback Method
log10ws	-8.01		Crippen Method
logp	6.329		Crippen Method
mcvol	309.370	ml/mol	McGowan Method
pc	1207.31	kPa	Joback Method
rinpol	3105.00		NIST Webbook
rinpol	3105.00		NIST Webbook
tb	940.37	K	Joback Method
tc	1154.33	K	Joback Method
tf	588.47	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	983.45	J/mol×K	940.37	Joback Method
cpg	996.46	J/mol×K	976.03	Joback Method
cpg	1008.29	J/mol×K	1011.69	Joback Method
cpg	1018.99	J/mol×K	1047.35	Joback Method
cpg	1028.61	J/mol×K	1083.01	Joback Method
cpg	1037.23	J/mol×K	1118.67	Joback Method
cpg	1044.88	J/mol×K	1154.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382948&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