Terephthalic acid, heptyl 4-trifluoromethoxybenzyl ester

Inchi: InChI=1S/C23H25F3O5/c1-2-3-4-5-6-15-29-21(27)18-9-11-19(12-10-18)22(28)30-16-17-

InchiKey: QRADQWOAFLOSGC-UHFFFAOYSA-N

Formula: C23H25F3O5

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

Mol. weight [g/mol]: 438.44

Physical Properties

Property code	Value	Unit	Source
gf	-806.09	kJ/mol	Joback Method
hf	-1286.83	kJ/mol	Joback Method
hfus	51.22	kJ/mol	Joback Method
hvap	89.64	kJ/mol	Joback Method
log10ws	-7.86		Crippen Method
logp	6.069		Crippen Method
mcvol	313.470	ml/mol	McGowan Method
pc	1244.21	kPa	Joback Method
rinpol	2884.00		NIST Webbook
rinpol	2884.00		NIST Webbook
tb	958.54	K	Joback Method
tc	1176.69	K	Joback Method
tf	597.59	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1004.68	J/mol×K	958.54	Joback Method
cpg	1017.34	J/mol×K	994.90	Joback Method
cpg	1028.68	J/mol×K	1031.26	Joback Method
cpg	1038.75	J/mol×K	1067.62	Joback Method
cpg	1047.59	J/mol×K	1103.97	Joback Method
cpg	1055.27	J/mol×K	1140.33	Joback Method
cpg	1061.82	J/mol×K	1176.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415979&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

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