Terephthalic acid, di(4-trifluoromethoxybenzyl) ester

Inchi: InChI=1S/C24H16F6O6/c25-23(26,27)35-19-9-1-15(2-10-19)13-33-21(31)17-5-7-18(8-6-

InchiKey: DWLQRKMEBGXRFF-UHFFFAOYSA-N

Formula: C24H16F6O6

SMILES: O=C(OCc1ccc(OC(F)(F)F)cc1)c1ccc(C(=O)OCc2ccc(OC(F)(F)F)cc2)cc1

Mol. weight [g/mol]: 514.37

Physical Properties

Property code	Value	Unit	Source
gf	-1381.48	kJ/mol	Joback Method
hf	-1811.71	kJ/mol	Joback Method
hfus	50.47	kJ/mol	Joback Method
hvap	93.47	kJ/mol	Joback Method
log10ws	-8.73		Crippen Method
logp	6.198		Crippen Method
mcvol	314.980	ml/mol	McGowan Method
pc	1324.24	kPa	Joback Method
rinpol	2101.00		NIST Webbook
rinpol	2101.00		NIST Webbook
tb	1030.08	K	Joback Method
tc	1263.26	K	Joback Method
tf	674.22	K	Joback Method
vc	1.226	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.64	J/mol×K	1030.08	Joback Method
cpg	1005.99	J/mol×K	1068.94	Joback Method
cpg	1013.02	J/mol×K	1107.81	Joback Method
cpg	1018.78	J/mol×K	1146.67	Joback Method
cpg	1023.37	J/mol×K	1185.53	Joback Method
cpg	1026.85	J/mol×K	1224.40	Joback Method
cpg	1029.30	J/mol×K	1263.26	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=U415981&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