Terephthalic acid, hexyl 4-(trifluoromethyl)benzyl ester

Inchi: InChI=1S/C22H23F3O4/c1-2-3-4-5-14-28-20(26)17-8-10-18(11-9-17)21(27)29-15-16-6-1

InchiKey: IPTCXVTUVBYCMS-UHFFFAOYSA-N

Formula: C22H23F3O4

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

Mol. weight [g/mol]: 408.41

Physical Properties

Property code	Value	Unit	Source
gf	-709.51	kJ/mol	Joback Method
hf	-1133.97	kJ/mol	Joback Method
hfus	47.44	kJ/mol	Joback Method
hvap	85.01	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	5.800		Crippen Method
mcvol	293.510	ml/mol	McGowan Method
pc	1349.66	kPa	Joback Method
rinpol	3018.00		NIST Webbook
rinpol	3018.00		NIST Webbook
tb	913.24	K	Joback Method
tc	1127.48	K	Joback Method
tf	564.09	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.82	J/mol×K	913.24	Joback Method
cpg	932.03	J/mol×K	948.95	Joback Method
cpg	944.08	J/mol×K	984.65	Joback Method
cpg	955.02	J/mol×K	1020.36	Joback Method
cpg	964.91	J/mol×K	1056.07	Joback Method
cpg	973.81	J/mol×K	1091.77	Joback Method
cpg	981.78	J/mol×K	1127.48	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=U383033&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