Terephthalic acid, heptyl 2,2,2-trifluoro-1-phenylethyl ester

Inchi: InChI=1S/C23H25F3O4/c1-2-3-4-5-9-16-29-21(27)18-12-14-19(15-13-18)22(28)30-20(23

InchiKey: YBSGMZLPYBGLBU-UHFFFAOYSA-N

Formula: C23H25F3O4

SMILES: CCCCCCCOC(=O)c1ccc(C(=O)OC(c2ccccc2)C(F)(F)F)cc1

Mol. weight [g/mol]: 422.44

Physical Properties

Property code	Value	Unit	Source
gf	-693.90	kJ/mol	Joback Method
hf	-1148.42	kJ/mol	Joback Method
hfus	46.90	kJ/mol	Joback Method
hvap	86.18	kJ/mol	Joback Method
log10ws	-7.62		Crippen Method
logp	6.274		Crippen Method
mcvol	307.600	ml/mol	McGowan Method
pc	1280.08	kPa	Joback Method
rinpol	2714.00		NIST Webbook
rinpol	2714.00		NIST Webbook
tb	930.70	K	Joback Method
tc	1146.78	K	Joback Method
tf	547.84	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	979.13	J/mol×K	930.70	Joback Method
cpg	992.66	J/mol×K	966.71	Joback Method
cpg	1004.98	J/mol×K	1002.73	Joback Method
cpg	1016.16	J/mol×K	1038.74	Joback Method
cpg	1026.28	J/mol×K	1074.75	Joback Method
cpg	1035.41	J/mol×K	1110.76	Joback Method
cpg	1043.60	J/mol×K	1146.78	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=U415988&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