Terephthalic acid, dodecyl 2,2,2-trifluoroethyl ester

Inchi: InChI=1S/C22H31F3O4/c1-2-3-4-5-6-7-8-9-10-11-16-28-20(26)18-12-14-19(15-13-18)21

InchiKey: CUGLLRYNVYEFBF-UHFFFAOYSA-N

Formula: C22H31F3O4

SMILES: CCCCCCCCCCCCOC(=O)c1ccc(C(=O)OCC(F)(F)F)cc1

Mol. weight [g/mol]: 416.47

Physical Properties

Property code	Value	Unit	Source
gf	-812.29	kJ/mol	Joback Method
hf	-1359.03	kJ/mol	Joback Method
hfus	53.79	kJ/mol	Joback Method
hvap	82.07	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	6.483		Crippen Method
mcvol	317.270	ml/mol	McGowan Method
pc	1083.49	kPa	Joback Method
rinpol	2740.00		NIST Webbook
rinpol	2740.00		NIST Webbook
tb	881.58	K	Joback Method
tc	1080.54	K	Joback Method
tf	525.15	K	Joback Method
vc	1.250	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1019.44	J/mol×K	881.58	Joback Method
cpg	1035.16	J/mol×K	914.74	Joback Method
cpg	1049.75	J/mol×K	947.90	Joback Method
cpg	1063.24	J/mol×K	981.06	Joback Method
cpg	1075.70	J/mol×K	1014.22	Joback Method
cpg	1087.16	J/mol×K	1047.38	Joback Method
cpg	1097.67	J/mol×K	1080.54	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=U383047&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