Terephthalic acid, decyl 2,2,3,3,4,4,4-heptafluorobutyl ester

Inchi: InChI=1S/C22H27F7O4/c1-2-3-4-5-6-7-8-9-14-32-18(30)16-10-12-17(13-11-16)19(31)33
InchiKey: HEQGLWRGMHKLME-UHFFFAOYSA-N
Formula: C22H27F7O4
SMILES: CCCCCCCCCCOC(=O)c1ccc(C(=O)OCC(F)(F)C(F)(F)C(F)(F)F)cc1
Mol. weight [g/mol]: 488.44

Physical Properties

Property code	Value	Unit	Source
gf	-1585.85	kJ/mol	Joback Method
hf	-2160.97	kJ/mol	Joback Method
hfus	51.28	kJ/mol	Joback Method
hvap	76.21	kJ/mol	Joback Method
log10ws	-8.27		Crippen Method
logp	6.974		Crippen Method
mcvol	324.350	ml/mol	McGowan Method
pc	988.88	kPa	Joback Method
rinpol	2408.00		NIST Webbook
rinpol	2408.00		NIST Webbook
tb	872.20	K	Joback Method
tc	1067.96	K	Joback Method
tf	532.35	K	Joback Method
vc	1.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1049.79	J/mol×K	872.20	Joback Method
cpg	1064.46	J/mol×K	904.83	Joback Method
cpg	1078.11	J/mol×K	937.45	Joback Method
cpg	1090.81	J/mol×K	970.08	Joback Method
cpg	1102.65	J/mol×K	1002.71	Joback Method
cpg	1113.70	J/mol×K	1035.34	Joback Method
cpg	1124.05	J/mol×K	1067.96	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415944&Units=SI

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