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

Inchi: InChI=1S/C23H29F7O4/c1-2-3-4-5-6-7-8-9-10-15-33-19(31)17-11-13-18(14-12-17)20(32

InchiKey: FBJCKJUMXNADJF-UHFFFAOYSA-N

Formula: C23H29F7O4

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

Mol. weight [g/mol]: 502.46

Physical Properties

Property code	Value	Unit	Source
gf	-1577.43	kJ/mol	Joback Method
hf	-2181.61	kJ/mol	Joback Method
hfus	53.87	kJ/mol	Joback Method
hvap	78.44	kJ/mol	Joback Method
log10ws	-8.69		Crippen Method
logp	7.364		Crippen Method
mcvol	338.440	ml/mol	McGowan Method
pc	931.78	kPa	Joback Method
rinpol	2503.00		NIST Webbook
rinpol	2503.00		NIST Webbook
tb	895.08	K	Joback Method
tc	1095.92	K	Joback Method
tf	543.62	K	Joback Method
vc	1.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1109.26	J/mol×K	895.08	Joback Method
cpg	1124.41	J/mol×K	928.55	Joback Method
cpg	1138.49	J/mol×K	962.03	Joback Method
cpg	1151.60	J/mol×K	995.50	Joback Method
cpg	1163.82	J/mol×K	1028.97	Joback Method
cpg	1175.23	J/mol×K	1062.45	Joback Method
cpg	1185.93	J/mol×K	1095.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415945&Units=SI
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

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