Terephthalic acid, 2,2,3,3,3-pentafluoropropyl octyl ester

Inchi: InChI=1S/C19H23F5O4/c1-2-3-4-5-6-7-12-27-16(25)14-8-10-15(11-9-14)17(26)28-13-18

InchiKey: SVVGSMOPKCUKFK-UHFFFAOYSA-N

Formula: C19H23F5O4

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

Mol. weight [g/mol]: 410.38

Physical Properties

Property code	Value	Unit	Source
gf	-1224.33	kJ/mol	Joback Method
hf	-1698.08	kJ/mol	Joback Method
hfus	44.76	kJ/mol	Joback Method
hvap	72.46	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	5.558		Crippen Method
mcvol	278.540	ml/mol	McGowan Method
pc	1256.59	kPa	Joback Method
rinpol	2180.00		NIST Webbook
rinpol	2180.00		NIST Webbook
tb	808.25	K	Joback Method
tc	996.82	K	Joback Method
tf	494.94	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	859.22	J/mol×K	808.25	Joback Method
cpg	873.32	J/mol×K	839.68	Joback Method
cpg	886.46	J/mol×K	871.11	Joback Method
cpg	898.68	J/mol×K	902.53	Joback Method
cpg	910.04	J/mol×K	933.96	Joback Method
cpg	920.59	J/mol×K	965.39	Joback Method
cpg	930.37	J/mol×K	996.82	Joback Method

Sources

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=U415779&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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