Terephthalic acid, heptyl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C19H22F6O4/c1-2-3-4-5-6-11-28-15(26)13-7-9-14(10-8-13)16(27)29-12-18(21
InchiKey: DHUCEWFZXGWHCK-UHFFFAOYSA-N
Formula: C19H22F6O4
SMILES: CCCCCCCOC(=O)c1ccc(C(=O)OCC(F)(F)C(F)C(F)(F)F)cc1
Mol. weight [g/mol]: 428.37

Physical Properties

Property code	Value	Unit	Source
gf	-1421.58	kJ/mol	Joback Method
hf	-1899.47	kJ/mol	Joback Method
hfus	44.32	kJ/mol	Joback Method
hvap	71.26	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	5.506		Crippen Method
mcvol	280.310	ml/mol	McGowan Method
pc	1224.27	kPa	Joback Method
rinpol	2325.00		NIST Webbook
tb	807.08	K	Joback Method
tc	993.83	K	Joback Method
tf	480.53	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	867.29	J/mol×K	807.08	Joback Method
cpg	881.16	J/mol×K	838.21	Joback Method
cpg	894.07	J/mol×K	869.33	Joback Method
cpg	906.08	J/mol×K	900.46	Joback Method
cpg	917.22	J/mol×K	931.58	Joback Method
cpg	927.55	J/mol×K	962.71	Joback Method
cpg	937.12	J/mol×K	993.83	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=U415754&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