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

Inchi: InChI=1S/C21H26F6O4/c1-2-3-4-5-6-7-8-13-30-17(28)15-9-11-16(12-10-15)18(29)31-14

InchiKey: VIMZVXBNLDIJHS-UHFFFAOYSA-N

Formula: C21H26F6O4

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

Mol. weight [g/mol]: 456.42

Physical Properties

Property code	Value	Unit	Source
gf	-1404.74	kJ/mol	Joback Method
hf	-1940.75	kJ/mol	Joback Method
hfus	49.50	kJ/mol	Joback Method
hvap	75.71	kJ/mol	Joback Method
log10ws	-7.50		Crippen Method
logp	6.287		Crippen Method
mcvol	308.490	ml/mol	McGowan Method
pc	1074.98	kPa	Joback Method
rinpol	2517.00		NIST Webbook
tb	852.84	K	Joback Method
tc	1045.34	K	Joback Method
tf	503.07	K	Joback Method
vc	1.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	983.20	J/mol×K	852.84	Joback Method
cpg	997.81	J/mol×K	884.92	Joback Method
cpg	1011.39	J/mol×K	917.01	Joback Method
cpg	1023.98	J/mol×K	949.09	Joback Method
cpg	1035.66	J/mol×K	981.17	Joback Method
cpg	1046.48	J/mol×K	1013.25	Joback Method
cpg	1056.48	J/mol×K	1045.34	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=U415756&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