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

Inchi: InChI=1S/C15H14F6O4/c1-2-7-24-11(22)9-3-5-10(6-4-9)12(23)25-8-14(17,18)13(16)15(1

InchiKey: JKCHSDSPNYNMCO-UHFFFAOYSA-N

Formula: C15H14F6O4

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

Mol. weight [g/mol]: 372.26

Physical Properties

Property code	Value	Unit	Source
gf	-1455.26	kJ/mol	Joback Method
hf	-1816.91	kJ/mol	Joback Method
hfus	33.96	kJ/mol	Joback Method
hvap	62.35	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	3.946		Crippen Method
mcvol	223.950	ml/mol	McGowan Method
pc	1633.81	kPa	Joback Method
rinpol	1833.00		NIST Webbook
rinpol	1833.00		NIST Webbook
tb	715.56	K	Joback Method
tc	898.96	K	Joback Method
tf	435.45	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.20	J/mol×K	715.56	Joback Method
cpg	658.64	J/mol×K	746.13	Joback Method
cpg	670.23	J/mol×K	776.69	Joback Method
cpg	681.01	J/mol×K	807.26	Joback Method
cpg	691.01	J/mol×K	837.83	Joback Method
cpg	700.27	J/mol×K	868.40	Joback Method
cpg	708.82	J/mol×K	898.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415749&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