Phthalic acid, 2,2,3,3,4,4,4-heptafluorobutyl propyl ester

Inchi: InChI=1S/C15H13F7O4/c1-2-7-25-11(23)9-5-3-4-6-10(9)12(24)26-8-13(16,17)14(18,19)1

InchiKey: UROUPYRSZUIYIH-UHFFFAOYSA-N

Formula: C15H13F7O4

SMILES: CCCOC(=O)c1ccccc1C(=O)OCC(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 390.25

Physical Properties

Property code	Value	Unit	Source
gf	-1644.79	kJ/mol	Joback Method
hf	-2016.49	kJ/mol	Joback Method
hfus	33.15	kJ/mol	Joback Method
hvap	60.63	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.243		Crippen Method
mcvol	225.720	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
rinpol	1664.00		NIST Webbook
rinpol	1664.00		NIST Webbook
tb	712.04	K	Joback Method
tc	894.09	K	Joback Method
tf	453.46	K	Joback Method
vc	0.908	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.14	J/mol×K	712.04	Joback Method
cpg	668.19	J/mol×K	742.38	Joback Method
cpg	679.37	J/mol×K	772.72	Joback Method
cpg	689.73	J/mol×K	803.06	Joback Method
cpg	699.33	J/mol×K	833.41	Joback Method
cpg	708.21	J/mol×K	863.75	Joback Method
cpg	716.42	J/mol×K	894.09	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=U415540&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