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

Inchi: InChI=1S/C27H37F7O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-19-37-23(35)21-17-14-15-18

InchiKey: FVDGXPSBOPXQJF-UHFFFAOYSA-N

Formula: C27H37F7O4

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

Mol. weight [g/mol]: 558.57

Physical Properties

Property code	Value	Unit	Source
gf	-1543.75	kJ/mol	Joback Method
hf	-2264.17	kJ/mol	Joback Method
hfus	64.23	kJ/mol	Joback Method
hvap	87.34	kJ/mol	Joback Method
log10ws	-10.36		Crippen Method
logp	8.924		Crippen Method
mcvol	394.800	ml/mol	McGowan Method
pc	746.51	kPa	Joback Method
rinpol	2534.00		NIST Webbook
tb	986.60	K	Joback Method
tc	1218.38	K	Joback Method
tf	588.70	K	Joback Method
vc	1.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1353.38	J/mol×K	986.60	Joback Method
cpg	1371.02	J/mol×K	1025.23	Joback Method
cpg	1387.36	J/mol×K	1063.86	Joback Method
cpg	1402.56	J/mol×K	1102.49	Joback Method
cpg	1416.78	J/mol×K	1141.12	Joback Method
cpg	1430.15	J/mol×K	1179.75	Joback Method
cpg	1442.84	J/mol×K	1218.38	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=U415557&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