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

Inchi: InChI=1S/C26H35F7O4/c1-2-3-4-5-6-7-8-9-10-11-12-15-18-36-22(34)20-16-13-14-17-21

InchiKey: JKEKMZDDZOCJET-UHFFFAOYSA-N

Formula: C26H35F7O4

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

Mol. weight [g/mol]: 544.54

Physical Properties

Property code	Value	Unit	Source
gf	-1552.17	kJ/mol	Joback Method
hf	-2243.53	kJ/mol	Joback Method
hfus	61.64	kJ/mol	Joback Method
hvap	85.11	kJ/mol	Joback Method
log10ws	-9.94		Crippen Method
logp	8.534		Crippen Method
mcvol	380.710	ml/mol	McGowan Method
pc	787.27	kPa	Joback Method
rinpol	2802.00		NIST Webbook
tb	963.72	K	Joback Method
tc	1186.00	K	Joback Method
tf	577.43	K	Joback Method
vc	1.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1291.49	J/mol×K	963.72	Joback Method
cpg	1308.40	J/mol×K	1000.77	Joback Method
cpg	1324.08	J/mol×K	1037.81	Joback Method
cpg	1338.67	J/mol×K	1074.86	Joback Method
cpg	1352.29	J/mol×K	1111.91	Joback Method
cpg	1365.08	J/mol×K	1148.95	Joback Method
cpg	1377.16	J/mol×K	1186.00	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=U415552&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