Phthalic acid, decyl 2,2,2-trifluoro-1-phenylethyl ester

Inchi: InChI=1S/C26H31F3O4/c1-2-3-4-5-6-7-8-14-19-32-24(30)21-17-12-13-18-22(21)25(31)3

InchiKey: GTCCPYJZRRHZPZ-UHFFFAOYSA-N

Formula: C26H31F3O4

SMILES: CCCCCCCCCCOC(=O)c1ccccc1C(=O)OC(c1ccccc1)C(F)(F)F

Mol. weight [g/mol]: 464.52

Physical Properties

Property code	Value	Unit	Source
gf	-668.64	kJ/mol	Joback Method
hf	-1210.34	kJ/mol	Joback Method
hfus	54.67	kJ/mol	Joback Method
hvap	92.86	kJ/mol	Joback Method
log10ws	-8.88		Crippen Method
logp	7.444		Crippen Method
mcvol	349.870	ml/mol	McGowan Method
pc	1052.09	kPa	Joback Method
rinpol	2798.00		NIST Webbook
rinpol	2798.00		NIST Webbook
tb	999.34	K	Joback Method
tc	1223.84	K	Joback Method
tf	581.65	K	Joback Method
vc	1.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1158.60	J/mol×K	999.34	Joback Method
cpg	1172.69	J/mol×K	1036.76	Joback Method
cpg	1185.48	J/mol×K	1074.17	Joback Method
cpg	1197.06	J/mol×K	1111.59	Joback Method
cpg	1207.51	J/mol×K	1149.00	Joback Method
cpg	1216.94	J/mol×K	1186.42	Joback Method
cpg	1225.41	J/mol×K	1223.84	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=U377708&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