Phthalic acid, dodecyl 2,3,6-trifluorobenzyl ester

Inchi: InChI=1S/C27H33F3O4/c1-2-3-4-5-6-7-8-9-10-13-18-33-26(31)20-14-11-12-15-21(20)27

InchiKey: DGPAGXNNNBIMCV-UHFFFAOYSA-N

Formula: C27H33F3O4

SMILES: CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1c(F)ccc(F)c1F

Mol. weight [g/mol]: 478.54

Physical Properties

Property code	Value	Unit	Source
gf	-689.51	kJ/mol	Joback Method
hf	-1251.36	kJ/mol	Joback Method
hfus	67.03	kJ/mol	Joback Method
hvap	98.76	kJ/mol	Joback Method
log10ws	-9.67		Crippen Method
logp	7.539		Crippen Method
mcvol	363.960	ml/mol	McGowan Method
pc	946.16	kPa	Joback Method
rinpol	3118.00		NIST Webbook
rinpol	3118.00		NIST Webbook
tb	1040.83	K	Joback Method
tc	1276.33	K	Joback Method
tf	643.06	K	Joback Method
vc	1.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1215.51	J/mol×K	1040.83	Joback Method
cpg	1229.32	J/mol×K	1080.08	Joback Method
cpg	1241.45	J/mol×K	1119.33	Joback Method
cpg	1251.98	J/mol×K	1158.58	Joback Method
cpg	1260.95	J/mol×K	1197.83	Joback Method
cpg	1268.41	J/mol×K	1237.08	Joback Method
cpg	1274.43	J/mol×K	1276.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377795&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