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

Inchi: InChI=1S/C26H31F3O4/c1-2-3-4-5-6-7-8-9-12-17-32-25(30)19-13-10-11-14-20(19)26(31

InchiKey: KHJPPSMWEJBJSP-UHFFFAOYSA-N

Formula: C26H31F3O4

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

Mol. weight [g/mol]: 464.52

Physical Properties

Property code	Value	Unit	Source
gf	-697.93	kJ/mol	Joback Method
hf	-1230.72	kJ/mol	Joback Method
hfus	64.44	kJ/mol	Joback Method
hvap	96.53	kJ/mol	Joback Method
log10ws	-9.25		Crippen Method
logp	7.149		Crippen Method
mcvol	349.870	ml/mol	McGowan Method
pc	1004.62	kPa	Joback Method
rinpol	3015.00		NIST Webbook
rinpol	3015.00		NIST Webbook
tb	1017.95	K	Joback Method
tc	1246.72	K	Joback Method
tf	631.79	K	Joback Method
vc	1.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1154.69	J/mol×K	1017.95	Joback Method
cpg	1168.31	J/mol×K	1056.08	Joback Method
cpg	1180.38	J/mol×K	1094.21	Joback Method
cpg	1190.93	J/mol×K	1132.33	Joback Method
cpg	1200.02	J/mol×K	1170.46	Joback Method
cpg	1207.69	J/mol×K	1208.59	Joback Method
cpg	1213.99	J/mol×K	1246.72	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=U377794&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