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

Inchi: InChI=1S/C25H29F3O4/c1-2-3-4-5-6-7-8-11-16-31-24(29)18-12-9-10-13-19(18)25(30)32
InchiKey: JIVGOKSNLUUBTO-UHFFFAOYSA-N
Formula: C25H29F3O4
SMILES: CCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1c(F)ccc(F)c1F
Mol. weight [g/mol]: 450.49

Physical Properties

Property code	Value	Unit	Source
gf	-706.35	kJ/mol	Joback Method
hf	-1210.08	kJ/mol	Joback Method
hfus	61.85	kJ/mol	Joback Method
hvap	94.30	kJ/mol	Joback Method
log10ws	-8.83		Crippen Method
logp	6.758		Crippen Method
mcvol	335.780	ml/mol	McGowan Method
pc	1068.66	kPa	Joback Method
rinpol	2915.00		NIST Webbook
rinpol	2915.00		NIST Webbook
tb	995.07	K	Joback Method
tc	1218.25	K	Joback Method
tf	620.52	K	Joback Method
vc	1.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1094.27	J/mol×K	995.07	Joback Method
cpg	1107.71	J/mol×K	1032.27	Joback Method
cpg	1119.70	J/mol×K	1069.46	Joback Method
cpg	1130.26	J/mol×K	1106.66	Joback Method
cpg	1139.44	J/mol×K	1143.86	Joback Method
cpg	1147.27	J/mol×K	1181.05	Joback Method
cpg	1153.81	J/mol×K	1218.25	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=U377793&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