Phthalic acid, hept-2-yl 2,4,5-trifluorobenzyl ester

Inchi: InChI=1S/C22H23F3O4/c1-3-4-5-8-14(2)29-22(27)17-10-7-6-9-16(17)21(26)28-13-15-11
InchiKey: NNNIGNNTFPLQCD-UHFFFAOYSA-N
Formula: C22H23F3O4
SMILES: CCCCCC(C)OC(=O)c1ccccc1C(=O)OCc1cc(F)c(F)cc1F
Mol. weight [g/mol]: 408.41

Physical Properties

Property code	Value	Unit	Source
gf	-734.05	kJ/mol	Joback Method
hf	-1153.44	kJ/mol	Joback Method
hfus	50.55	kJ/mol	Joback Method
hvap	87.24	kJ/mol	Joback Method
log10ws	-7.68		Crippen Method
logp	5.586		Crippen Method
mcvol	293.510	ml/mol	McGowan Method
pc	1309.90	kPa	Joback Method
rinpol	2563.00		NIST Webbook
rinpol	2563.00		NIST Webbook
tb	925.99	K	Joback Method
tc	1139.66	K	Joback Method
tf	571.71	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.37	J/mol×K	925.99	Joback Method
cpg	929.34	J/mol×K	961.60	Joback Method
cpg	941.04	J/mol×K	997.21	Joback Method
cpg	951.50	J/mol×K	1032.82	Joback Method
cpg	960.75	J/mol×K	1068.44	Joback Method
cpg	968.80	J/mol×K	1104.05	Joback Method
cpg	975.69	J/mol×K	1139.66	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=U415495&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