Phthalic acid, di(4-fluorobenzyl) ester

Inchi: InChI=1S/C22H16F2O4/c23-17-9-5-15(6-10-17)13-27-21(25)19-3-1-2-4-20(19)22(26)28-
InchiKey: LUFIBCXJLIJZMJ-UHFFFAOYSA-N
Formula: C22H16F2O4
SMILES: O=C(OCc1ccc(F)cc1)c1ccccc1C(=O)OCc1ccc(F)cc1
Mol. weight [g/mol]: 382.36

Physical Properties

Property code	Value	Unit	Source
gf	-414.76	kJ/mol	Joback Method
hf	-704.05	kJ/mol	Joback Method
hfus	45.43	kJ/mol	Joback Method
hvap	90.06	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	4.679		Crippen Method
mcvol	267.980	ml/mol	McGowan Method
pc	1765.41	kPa	Joback Method
rinpol	3774.00		NIST Webbook
tb	948.86	K	Joback Method
tc	1185.72	K	Joback Method
tf	600.02	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.89	J/mol×K	948.86	Joback Method
cpg	815.84	J/mol×K	988.34	Joback Method
cpg	825.43	J/mol×K	1027.81	Joback Method
cpg	833.71	J/mol×K	1067.29	Joback Method
cpg	840.73	J/mol×K	1106.76	Joback Method
cpg	846.55	J/mol×K	1146.24	Joback Method
cpg	851.20	J/mol×K	1185.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377755&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