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

Inchi: InChI=1S/C21H21F3O4/c1-2-3-4-7-12-27-20(25)14-8-5-6-9-15(14)21(26)28-13-16-17(22
InchiKey: AHLBHDMOPCCZJX-UHFFFAOYSA-N
Formula: C21H21F3O4
SMILES: CCCCCCOC(=O)c1ccccc1C(=O)OCc1c(F)ccc(F)c1F
Mol. weight [g/mol]: 394.38

Physical Properties

Property code	Value	Unit	Source
gf	-740.03	kJ/mol	Joback Method
hf	-1127.52	kJ/mol	Joback Method
hfus	51.49	kJ/mol	Joback Method
hvap	85.40	kJ/mol	Joback Method
log10ws	-7.15		Crippen Method
logp	5.198		Crippen Method
mcvol	279.420	ml/mol	McGowan Method
pc	1397.50	kPa	Joback Method
rinpol	2520.00		NIST Webbook
rinpol	2520.00		NIST Webbook
tb	903.55	K	Joback Method
tc	1114.31	K	Joback Method
tf	575.44	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	857.56	J/mol×K	903.55	Joback Method
cpg	870.32	J/mol×K	938.68	Joback Method
cpg	881.90	J/mol×K	973.80	Joback Method
cpg	892.31	J/mol×K	1008.93	Joback Method
cpg	901.59	J/mol×K	1044.06	Joback Method
cpg	909.74	J/mol×K	1079.18	Joback Method
cpg	916.79	J/mol×K	1114.31	Joback Method

Sources

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=U377790&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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