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

Inchi: InChI=1S/C22H23F3O4/c1-2-3-4-5-8-13-28-21(26)15-9-6-7-10-16(15)22(27)29-14-17-18
InchiKey: AKODANXSUACKPU-UHFFFAOYSA-N
Formula: C22H23F3O4
SMILES: CCCCCCCOC(=O)c1ccccc1C(=O)OCc1c(F)ccc(F)c1F
Mol. weight [g/mol]: 408.41

Physical Properties

Property code	Value	Unit	Source
gf	-731.61	kJ/mol	Joback Method
hf	-1148.16	kJ/mol	Joback Method
hfus	54.08	kJ/mol	Joback Method
hvap	87.63	kJ/mol	Joback Method
log10ws	-7.57		Crippen Method
logp	5.588		Crippen Method
mcvol	293.510	ml/mol	McGowan Method
pc	1302.35	kPa	Joback Method
rinpol	2621.00		NIST Webbook
tb	926.43	K	Joback Method
tc	1138.93	K	Joback Method
tf	586.71	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	915.88	J/mol×K	926.43	Joback Method
cpg	928.82	J/mol×K	961.85	Joback Method
cpg	940.51	J/mol×K	997.26	Joback Method
cpg	950.99	J/mol×K	1032.68	Joback Method
cpg	960.28	J/mol×K	1068.10	Joback Method
cpg	968.41	J/mol×K	1103.52	Joback Method
cpg	975.39	J/mol×K	1138.93	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=U377791&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