Terephthalic acid, 2-fluorobenzyl heptyl ester

Inchi: InChI=1S/C22H25FO4/c1-2-3-4-5-8-15-26-21(24)17-11-13-18(14-12-17)22(25)27-16-19-
InchiKey: MHJSUQQHHAALIR-UHFFFAOYSA-N
Formula: C22H25FO4
SMILES: CCCCCCCOC(=O)c1ccc(C(=O)OCc2ccccc2F)cc1
Mol. weight [g/mol]: 372.43

Physical Properties

Property code	Value	Unit	Source
gf	-322.73	kJ/mol	Joback Method
hf	-733.00	kJ/mol	Joback Method
hfus	48.69	kJ/mol	Joback Method
hvap	87.94	kJ/mol	Joback Method
log10ws	-6.91		Crippen Method
logp	5.310		Crippen Method
mcvol	289.970	ml/mol	McGowan Method
pc	1422.92	kPa	Joback Method
rinpol	3212.00		NIST Webbook
rinpol	3212.00		NIST Webbook
tb	917.93	K	Joback Method
tc	1135.73	K	Joback Method
tf	560.49	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	903.90	J/mol×K	917.93	Joback Method
cpg	917.71	J/mol×K	954.23	Joback Method
cpg	930.24	J/mol×K	990.53	Joback Method
cpg	941.53	J/mol×K	1026.83	Joback Method
cpg	951.60	J/mol×K	1063.13	Joback Method
cpg	960.51	J/mol×K	1099.43	Joback Method
cpg	968.28	J/mol×K	1135.73	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=U383015&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