Terephthalic acid, 2-fluoroethyl pentyl ester

Inchi: InChI=1S/C15H19FO4/c1-2-3-4-10-19-14(17)12-5-7-13(8-6-12)15(18)20-11-9-16/h5-8H,2
InchiKey: VESTXGCUCVJZCC-UHFFFAOYSA-N
Formula: C15H19FO4
SMILES: CCCCCOC(=O)c1ccc(C(=O)OCCF)cc1
Mol. weight [g/mol]: 282.31

Physical Properties

Property code	Value	Unit	Source
gf	-484.45	kJ/mol	Joback Method
hf	-813.58	kJ/mol	Joback Method
hfus	36.91	kJ/mol	Joback Method
hvap	69.42	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.160		Crippen Method
mcvol	215.100	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	2236.00		NIST Webbook
rinpol	2236.00		NIST Webbook
tb	726.11	K	Joback Method
tc	922.73	K	Joback Method
tf	442.66	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.45	J/mol×K	726.11	Joback Method
cpg	615.65	J/mol×K	758.88	Joback Method
cpg	628.97	J/mol×K	791.65	Joback Method
cpg	641.42	J/mol×K	824.42	Joback Method
cpg	653.01	J/mol×K	857.19	Joback Method
cpg	663.75	J/mol×K	889.96	Joback Method
cpg	673.66	J/mol×K	922.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415792&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