Terephthalic acid, 2-fluoroethyl heptyl ester

Inchi: InChI=1S/C17H23FO4/c1-2-3-4-5-6-12-21-16(19)14-7-9-15(10-8-14)17(20)22-13-11-18/h
InchiKey: VRYZBDYCLKDSMR-UHFFFAOYSA-N
Formula: C17H23FO4
SMILES: CCCCCCCOC(=O)c1ccc(C(=O)OCCF)cc1
Mol. weight [g/mol]: 310.36

Physical Properties

Property code	Value	Unit	Source
gf	-467.61	kJ/mol	Joback Method
hf	-854.86	kJ/mol	Joback Method
hfus	42.09	kJ/mol	Joback Method
hvap	73.87	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.940		Crippen Method
mcvol	243.280	ml/mol	McGowan Method
pc	1616.77	kPa	Joback Method
rinpol	2445.00		NIST Webbook
rinpol	2445.00		NIST Webbook
tb	771.87	K	Joback Method
tc	966.58	K	Joback Method
tf	465.20	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.99	J/mol×K	771.87	Joback Method
cpg	726.89	J/mol×K	804.32	Joback Method
cpg	740.82	J/mol×K	836.77	Joback Method
cpg	753.82	J/mol×K	869.23	Joback Method
cpg	765.88	J/mol×K	901.68	Joback Method
cpg	777.03	J/mol×K	934.13	Joback Method
cpg	787.29	J/mol×K	966.58	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=U415794&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