Terephthalic acid, 4-fluorophenethyl octyl ester

Inchi: InChI=1S/C24H29FO4/c1-2-3-4-5-6-7-17-28-23(26)20-10-12-21(13-11-20)24(27)29-18-1
InchiKey: KOENKSMOAUCOMA-UHFFFAOYSA-N
Formula: C24H29FO4
SMILES: CCCCCCCCOC(=O)c1ccc(C(=O)OCCc2ccc(F)cc2)cc1
Mol. weight [g/mol]: 400.48

Physical Properties

Property code	Value	Unit	Source
gf	-305.89	kJ/mol	Joback Method
hf	-774.28	kJ/mol	Joback Method
hfus	53.87	kJ/mol	Joback Method
hvap	92.39	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	5.742		Crippen Method
mcvol	318.150	ml/mol	McGowan Method
pc	1237.22	kPa	Joback Method
rinpol	3127.00		NIST Webbook
rinpol	3127.00		NIST Webbook
tb	963.69	K	Joback Method
tc	1184.18	K	Joback Method
tf	583.03	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1022.64	J/mol×K	963.69	Joback Method
cpg	1036.65	J/mol×K	1000.44	Joback Method
cpg	1049.29	J/mol×K	1037.19	Joback Method
cpg	1060.60	J/mol×K	1073.94	Joback Method
cpg	1070.64	J/mol×K	1110.68	Joback Method
cpg	1079.45	J/mol×K	1147.43	Joback Method
cpg	1087.07	J/mol×K	1184.18	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=U416147&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