Terephthalic acid, di(2-fluorophenethyl) ester

Inchi: InChI=1S/C24H20F2O4/c25-21-7-3-1-5-17(21)13-15-29-23(27)19-9-11-20(12-10-19)24(2
InchiKey: IZQQJBFIKHVFAL-UHFFFAOYSA-N
Formula: C24H20F2O4
SMILES: O=C(OCCc1ccccc1F)c1ccc(C(=O)OCCc2ccccc2F)cc1
Mol. weight [g/mol]: 410.41

Physical Properties

Property code	Value	Unit	Source
gf	-397.92	kJ/mol	Joback Method
hf	-745.33	kJ/mol	Joback Method
hfus	50.61	kJ/mol	Joback Method
hvap	94.51	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	4.764		Crippen Method
mcvol	296.160	ml/mol	McGowan Method
pc	1511.67	kPa	Joback Method
rinpol	2381.00		NIST Webbook
rinpol	2381.00		NIST Webbook
tb	994.62	K	Joback Method
tc	1230.14	K	Joback Method
tf	622.56	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	920.40	J/mol×K	994.62	Joback Method
cpg	931.41	J/mol×K	1033.87	Joback Method
cpg	941.02	J/mol×K	1073.13	Joback Method
cpg	949.30	J/mol×K	1112.38	Joback Method
cpg	956.30	J/mol×K	1151.63	Joback Method
cpg	962.08	J/mol×K	1190.88	Joback Method
cpg	966.69	J/mol×K	1230.14	Joback Method

Sources

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=U416139&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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