Terephthalic acid, decyl 4-fluorophenethyl ester

Inchi: InChI=1S/C26H33FO4/c1-2-3-4-5-6-7-8-9-19-30-25(28)22-12-14-23(15-13-22)26(29)31-2

InchiKey: KXTCFHCOCPKBDE-UHFFFAOYSA-N

Formula: C26H33FO4

SMILES: CCCCCCCCCCOC(=O)c1ccc(C(=O)OCCc2ccc(F)cc2)cc1

Mol. weight [g/mol]: 428.54

Physical Properties

Property code	Value	Unit	Source
gf	-289.05	kJ/mol	Joback Method
hf	-815.56	kJ/mol	Joback Method
hfus	59.05	kJ/mol	Joback Method
hvap	96.84	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	6.523		Crippen Method
mcvol	346.330	ml/mol	McGowan Method
pc	1085.63	kPa	Joback Method
rinpol	2282.00		NIST Webbook
rinpol	2282.00		NIST Webbook
tb	1009.45	K	Joback Method
tc	1236.29	K	Joback Method
tf	605.57	K	Joback Method
vc	1.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1143.46	J/mol×K	1009.45	Joback Method
cpg	1157.69	J/mol×K	1047.26	Joback Method
cpg	1170.43	J/mol×K	1085.06	Joback Method
cpg	1181.74	J/mol×K	1122.87	Joback Method
cpg	1191.68	J/mol×K	1160.67	Joback Method
cpg	1200.32	J/mol×K	1198.48	Joback Method
cpg	1207.70	J/mol×K	1236.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416149&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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