Terephthalic acid, pentadecyl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C26H37F5O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-19-34-23(32)21-15-17-22(18

InchiKey: RTIRRUPGGGDSSV-UHFFFAOYSA-N

Formula: C26H37F5O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)c1ccc(C(=O)OCC(F)(F)C(F)(F)F)cc1

Mol. weight [g/mol]: 508.56

Physical Properties

Property code	Value	Unit	Source
gf	-1165.39	kJ/mol	Joback Method
hf	-1842.56	kJ/mol	Joback Method
hfus	62.89	kJ/mol	Joback Method
hvap	88.04	kJ/mol	Joback Method
log10ws	-9.63		Crippen Method
logp	8.289		Crippen Method
mcvol	377.170	ml/mol	McGowan Method
pc	819.60	kPa	Joback Method
rinpol	2866.00		NIST Webbook
rinpol	2866.00		NIST Webbook
tb	968.41	K	Joback Method
tc	1190.01	K	Joback Method
tf	573.83	K	Joback Method
vc	1.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1277.72	J/mol×K	968.41	Joback Method
cpg	1294.85	J/mol×K	1005.34	Joback Method
cpg	1310.65	J/mol×K	1042.28	Joback Method
cpg	1325.22	J/mol×K	1079.21	Joback Method
cpg	1338.67	J/mol×K	1116.15	Joback Method
cpg	1351.11	J/mol×K	1153.08	Joback Method
cpg	1362.63	J/mol×K	1190.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415786&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