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

Inchi: InChI=1S/C25H35F5O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-18-33-22(31)20-14-16-21(17-15

InchiKey: GWONAVIVCYKMFT-UHFFFAOYSA-N

Formula: C25H35F5O4

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

Mol. weight [g/mol]: 494.54

Physical Properties

Property code	Value	Unit	Source
gf	-1173.81	kJ/mol	Joback Method
hf	-1821.92	kJ/mol	Joback Method
hfus	60.30	kJ/mol	Joback Method
hvap	85.82	kJ/mol	Joback Method
log10ws	-9.21		Crippen Method
logp	7.899		Crippen Method
mcvol	363.080	ml/mol	McGowan Method
pc	866.58	kPa	Joback Method
rinpol	2765.00		NIST Webbook
rinpol	2765.00		NIST Webbook
tb	945.53	K	Joback Method
tc	1159.44	K	Joback Method
tf	562.56	K	Joback Method
vc	1.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1216.06	J/mol×K	945.53	Joback Method
cpg	1232.63	J/mol×K	981.18	Joback Method
cpg	1247.95	J/mol×K	1016.83	Joback Method
cpg	1262.10	J/mol×K	1052.49	Joback Method
cpg	1275.19	J/mol×K	1088.14	Joback Method
cpg	1287.29	J/mol×K	1123.79	Joback Method
cpg	1298.50	J/mol×K	1159.44	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=U415785&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