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

Inchi: InChI=1S/C24H33F5O4/c1-2-3-4-5-6-7-8-9-10-11-12-17-32-21(30)19-13-15-20(16-14-19
InchiKey: LYVFVOQPINRPNI-UHFFFAOYSA-N
Formula: C24H33F5O4
SMILES: CCCCCCCCCCCCCOC(=O)c1ccc(C(=O)OCC(F)(F)C(F)(F)F)cc1
Mol. weight [g/mol]: 480.51

Physical Properties

Property code	Value	Unit	Source
gf	-1182.23	kJ/mol	Joback Method
hf	-1801.28	kJ/mol	Joback Method
hfus	57.71	kJ/mol	Joback Method
hvap	83.59	kJ/mol	Joback Method
log10ws	-8.79		Crippen Method
logp	7.509		Crippen Method
mcvol	348.990	ml/mol	McGowan Method
pc	917.72	kPa	Joback Method
rinpol	2663.00		NIST Webbook
rinpol	2663.00		NIST Webbook
tb	922.65	K	Joback Method
tc	1129.99	K	Joback Method
tf	551.29	K	Joback Method
vc	1.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1154.95	J/mol×K	922.65	Joback Method
cpg	1171.01	J/mol×K	957.21	Joback Method
cpg	1185.89	J/mol×K	991.76	Joback Method
cpg	1199.67	J/mol×K	1026.32	Joback Method
cpg	1212.42	J/mol×K	1060.88	Joback Method
cpg	1224.22	J/mol×K	1095.43	Joback Method
cpg	1235.15	J/mol×K	1129.99	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=U415784&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