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

Inchi: InChI=1S/C21H27F5O4/c1-2-3-4-5-6-7-8-9-14-29-18(27)16-10-12-17(13-11-16)19(28)30

InchiKey: DYPOCXLOCCYDSP-UHFFFAOYSA-N

Formula: C21H27F5O4

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

Mol. weight [g/mol]: 438.43

Physical Properties

Property code	Value	Unit	Source
gf	-1207.49	kJ/mol	Joback Method
hf	-1739.36	kJ/mol	Joback Method
hfus	49.94	kJ/mol	Joback Method
hvap	76.91	kJ/mol	Joback Method
log10ws	-7.54		Crippen Method
logp	6.338		Crippen Method
mcvol	306.720	ml/mol	McGowan Method
pc	1101.54	kPa	Joback Method
rinpol	2376.00		NIST Webbook
rinpol	2376.00		NIST Webbook
tb	854.01	K	Joback Method
tc	1047.55	K	Joback Method
tf	517.48	K	Joback Method
vc	1.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	975.34	J/mol×K	854.01	Joback Method
cpg	990.15	J/mol×K	886.27	Joback Method
cpg	1003.92	J/mol×K	918.52	Joback Method
cpg	1016.72	J/mol×K	950.78	Joback Method
cpg	1028.60	J/mol×K	983.04	Joback Method
cpg	1039.62	J/mol×K	1015.29	Joback Method
cpg	1049.84	J/mol×K	1047.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415781&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