Terephthalic acid, dodecyl 2,2,3,3,4,4,4-heptafluorobutyl ester

Inchi: InChI=1S/C24H31F7O4/c1-2-3-4-5-6-7-8-9-10-11-16-34-20(32)18-12-14-19(15-13-18)21

InchiKey: BREIHXBPUJZCAY-UHFFFAOYSA-N

Formula: C24H31F7O4

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

Mol. weight [g/mol]: 516.49

Physical Properties

Property code	Value	Unit	Source
gf	-1569.01	kJ/mol	Joback Method
hf	-2202.25	kJ/mol	Joback Method
hfus	56.46	kJ/mol	Joback Method
hvap	80.66	kJ/mol	Joback Method
log10ws	-9.11		Crippen Method
logp	7.754		Crippen Method
mcvol	352.530	ml/mol	McGowan Method
pc	879.48	kPa	Joback Method
rinpol	2798.00		NIST Webbook
rinpol	2798.00		NIST Webbook
tb	917.96	K	Joback Method
tc	1124.86	K	Joback Method
tf	554.89	K	Joback Method
vc	1.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1169.40	J/mol×K	917.96	Joback Method
cpg	1185.07	J/mol×K	952.44	Joback Method
cpg	1199.63	J/mol×K	986.93	Joback Method
cpg	1213.18	J/mol×K	1021.41	Joback Method
cpg	1225.81	J/mol×K	1055.89	Joback Method
cpg	1237.63	J/mol×K	1090.38	Joback Method
cpg	1248.74	J/mol×K	1124.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415946&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