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

Inchi: InChI=1S/C29H43F5O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22-37-26(35)24-18

InchiKey: GBFMQUBDBIDVDO-UHFFFAOYSA-N

Formula: C29H43F5O4

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

Mol. weight [g/mol]: 550.64

Physical Properties

Property code	Value	Unit	Source
gf	-1140.13	kJ/mol	Joback Method
hf	-1904.48	kJ/mol	Joback Method
hfus	70.66	kJ/mol	Joback Method
hvap	94.72	kJ/mol	Joback Method
log10ws	-10.89		Crippen Method
logp	9.459		Crippen Method
mcvol	419.440	ml/mol	McGowan Method
pc	699.50	kPa	Joback Method
rinpol	1814.00		NIST Webbook
rinpol	1814.00		NIST Webbook
tb	1037.05	K	Joback Method
tc	1289.34	K	Joback Method
tf	607.64	K	Joback Method
vc	1.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1465.62	J/mol×K	1037.05	Joback Method
cpg	1484.81	J/mol×K	1079.10	Joback Method
cpg	1502.38	J/mol×K	1121.15	Joback Method
cpg	1518.50	J/mol×K	1163.19	Joback Method
cpg	1533.34	J/mol×K	1205.24	Joback Method
cpg	1547.06	J/mol×K	1247.29	Joback Method
cpg	1559.84	J/mol×K	1289.34	Joback Method

Sources

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=U415788&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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