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

Inchi: InChI=1S/C28H39F7O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-20-38-24(36)22-16-18-23

InchiKey: WSCWVIYPVCHHRX-UHFFFAOYSA-N

Formula: C28H39F7O4

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

Mol. weight [g/mol]: 572.60

Physical Properties

Property code	Value	Unit	Source
gf	-1535.33	kJ/mol	Joback Method
hf	-2284.81	kJ/mol	Joback Method
hfus	66.82	kJ/mol	Joback Method
hvap	89.56	kJ/mol	Joback Method
log10ws	-10.78		Crippen Method
logp	9.314		Crippen Method
mcvol	408.890	ml/mol	McGowan Method
pc	708.84	kPa	Joback Method
rinpol	2992.00		NIST Webbook
rinpol	2992.00		NIST Webbook
tb	1009.48	K	Joback Method
tc	1252.09	K	Joback Method
tf	599.97	K	Joback Method
vc	1.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1415.79	J/mol×K	1009.48	Joback Method
cpg	1434.24	J/mol×K	1049.91	Joback Method
cpg	1451.33	J/mol×K	1090.35	Joback Method
cpg	1467.23	J/mol×K	1130.78	Joback Method
cpg	1482.12	J/mol×K	1171.22	Joback Method
cpg	1496.18	J/mol×K	1211.65	Joback Method
cpg	1509.59	J/mol×K	1252.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415948&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