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

Inchi: InChI=1S/C18H19F7O4/c1-2-3-4-5-10-28-14(26)12-6-8-13(9-7-12)15(27)29-11-16(19,20

InchiKey: OFSFVJSUESAENW-UHFFFAOYSA-N

Formula: C18H19F7O4

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

Mol. weight [g/mol]: 432.33

Physical Properties

Property code	Value	Unit	Source
gf	-1619.53	kJ/mol	Joback Method
hf	-2078.41	kJ/mol	Joback Method
hfus	40.92	kJ/mol	Joback Method
hvap	67.31	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	5.413		Crippen Method
mcvol	267.990	ml/mol	McGowan Method
pc	1279.16	kPa	Joback Method
rinpol	2030.00		NIST Webbook
rinpol	2030.00		NIST Webbook
tb	780.68	K	Joback Method
tc	964.55	K	Joback Method
tf	487.27	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.45	J/mol×K	780.68	Joback Method
cpg	832.56	J/mol×K	811.32	Joback Method
cpg	844.75	J/mol×K	841.97	Joback Method
cpg	856.09	J/mol×K	872.61	Joback Method
cpg	866.63	J/mol×K	903.26	Joback Method
cpg	876.44	J/mol×K	933.90	Joback Method
cpg	885.56	J/mol×K	964.55	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=U415940&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