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

Inchi: InChI=1S/C17H19F5O4/c1-2-3-4-5-10-25-14(23)12-6-8-13(9-7-12)15(24)26-11-16(18,19

InchiKey: SXYABEMETNGUAK-UHFFFAOYSA-N

Formula: C17H19F5O4

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

Mol. weight [g/mol]: 382.32

Physical Properties

Property code	Value	Unit	Source
gf	-1241.17	kJ/mol	Joback Method
hf	-1656.80	kJ/mol	Joback Method
hfus	39.58	kJ/mol	Joback Method
hvap	68.01	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	4.778		Crippen Method
mcvol	250.360	ml/mol	McGowan Method
pc	1446.83	kPa	Joback Method
rinpol	1992.00		NIST Webbook
rinpol	1992.00		NIST Webbook
tb	762.49	K	Joback Method
tc	948.89	K	Joback Method
tf	472.40	K	Joback Method
vc	0.996	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.53	J/mol×K	762.49	Joback Method
cpg	759.95	J/mol×K	793.56	Joback Method
cpg	772.47	J/mol×K	824.62	Joback Method
cpg	784.12	J/mol×K	855.69	Joback Method
cpg	794.95	J/mol×K	886.76	Joback Method
cpg	805.00	J/mol×K	917.83	Joback Method
cpg	814.31	J/mol×K	948.89	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415777&Units=SI

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