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

Inchi: InChI=1S/C14H11F7O4/c1-2-24-10(22)8-3-5-9(6-4-8)11(23)25-7-12(15,16)13(17,18)14(1

InchiKey: CQVQIYBTYMVFTO-UHFFFAOYSA-N

Formula: C14H11F7O4

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

Mol. weight [g/mol]: 376.22

Physical Properties

Property code	Value	Unit	Source
gf	-1653.21	kJ/mol	Joback Method
hf	-1995.85	kJ/mol	Joback Method
hfus	30.56	kJ/mol	Joback Method
hvap	58.40	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	3.853		Crippen Method
mcvol	211.630	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
rinpol	1634.00		NIST Webbook
rinpol	1634.00		NIST Webbook
tb	689.16	K	Joback Method
tc	871.66	K	Joback Method
tf	442.19	K	Joback Method
vc	0.853	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.84	J/mol×K	689.16	Joback Method
cpg	615.50	J/mol×K	719.58	Joback Method
cpg	626.31	J/mol×K	749.99	Joback Method
cpg	636.31	J/mol×K	780.41	Joback Method
cpg	645.56	J/mol×K	810.83	Joback Method
cpg	654.09	J/mol×K	841.25	Joback Method
cpg	661.96	J/mol×K	871.66	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=U415935&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