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

Inchi: InChI=1S/C15H15F5O4/c1-2-3-8-23-12(21)10-4-6-11(7-5-10)13(22)24-9-14(16,17)15(18

InchiKey: FFFXDDUPDDWSFA-UHFFFAOYSA-N

Formula: C15H15F5O4

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

Mol. weight [g/mol]: 354.27

Physical Properties

Property code	Value	Unit	Source
gf	-1258.01	kJ/mol	Joback Method
hf	-1615.52	kJ/mol	Joback Method
hfus	34.40	kJ/mol	Joback Method
hvap	63.56	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	3.998		Crippen Method
mcvol	222.180	ml/mol	McGowan Method
pc	1683.79	kPa	Joback Method
rinpol	1785.00		NIST Webbook
rinpol	1785.00		NIST Webbook
tb	716.73	K	Joback Method
tc	903.33	K	Joback Method
tf	449.86	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.78	J/mol×K	716.73	Joback Method
cpg	650.49	J/mol×K	747.83	Joback Method
cpg	662.33	J/mol×K	778.93	Joback Method
cpg	673.35	J/mol×K	810.03	Joback Method
cpg	683.58	J/mol×K	841.13	Joback Method
cpg	693.06	J/mol×K	872.23	Joback Method
cpg	701.83	J/mol×K	903.33	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=U415775&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