Terephthalic acid, butyl 2,2,2-trifluoroethyl ester

Inchi: InChI=1S/C14H15F3O4/c1-2-3-8-20-12(18)10-4-6-11(7-5-10)13(19)21-9-14(15,16)17/h4-

InchiKey: VIPRVCQDHMFMRC-UHFFFAOYSA-N

Formula: C14H15F3O4

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

Mol. weight [g/mol]: 304.26

Physical Properties

Property code	Value	Unit	Source
gf	-879.65	kJ/mol	Joback Method
hf	-1193.91	kJ/mol	Joback Method
hfus	33.07	kJ/mol	Joback Method
hvap	64.26	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.363		Crippen Method
mcvol	204.550	ml/mol	McGowan Method
pc	1940.65	kPa	Joback Method
rinpol	1921.00		NIST Webbook
rinpol	1921.00		NIST Webbook
tb	698.54	K	Joback Method
tc	891.27	K	Joback Method
tf	434.99	K	Joback Method
vc	0.802	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.41	J/mol×K	698.54	Joback Method
cpg	579.43	J/mol×K	730.66	Joback Method
cpg	591.60	J/mol×K	762.78	Joback Method
cpg	602.96	J/mol×K	794.91	Joback Method
cpg	613.52	J/mol×K	827.03	Joback Method
cpg	623.32	J/mol×K	859.15	Joback Method
cpg	632.36	J/mol×K	891.27	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=U383039&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