Terephthalic acid, butyl 1-(pentafluorophenyl)ethyl ester

Inchi: InChI=1S/C20H17F5O4/c1-3-4-9-28-19(26)11-5-7-12(8-6-11)20(27)29-10(2)13-14(21)16
InchiKey: XAQOXOVBCJQKTH-UHFFFAOYSA-N
Formula: C20H17F5O4
SMILES: CCCCOC(=O)c1ccc(C(=O)OC(C)c2c(F)c(F)c(F)c(F)c2F)cc1
Mol. weight [g/mol]: 416.34

Physical Properties

Property code	Value	Unit	Source
gf	-1159.77	kJ/mol	Joback Method
hf	-1527.32	kJ/mol	Joback Method
hfus	50.76	kJ/mol	Joback Method
hvap	82.48	kJ/mol	Joback Method
log10ws	-7.36		Crippen Method
logp	5.257		Crippen Method
mcvol	268.870	ml/mol	McGowan Method
pc	1380.93	kPa	Joback Method
rinpol	2450.00		NIST Webbook
rinpol	2450.00		NIST Webbook
tb	888.73	K	Joback Method
tc	1094.42	K	Joback Method
tf	575.39	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.51	J/mol×K	888.73	Joback Method
cpg	824.31	J/mol×K	923.01	Joback Method
cpg	835.00	J/mol×K	957.29	Joback Method
cpg	844.59	J/mol×K	991.57	Joback Method
cpg	853.09	J/mol×K	1025.85	Joback Method
cpg	860.49	J/mol×K	1060.13	Joback Method
cpg	866.82	J/mol×K	1094.42	Joback Method

Sources

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=U416056&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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