4-Butylbenzoic acid, pentafluorophenyl ester

Inchi: InChI=1S/C17H13F5O2/c1-2-3-4-9-5-7-10(8-6-9)17(23)24-16-14(21)12(19)11(18)13(20)1
InchiKey: ZOEABCYVQXIGMA-UHFFFAOYSA-N
Formula: C17H13F5O2
SMILES: CCCCc1ccc(C(=O)Oc2c(F)c(F)c(F)c(F)c2F)cc1
Mol. weight [g/mol]: 344.28

Physical Properties

Property code	Value	Unit	Source
gf	-948.67	kJ/mol	Joback Method
hf	-1215.32	kJ/mol	Joback Method
hfus	43.72	kJ/mol	Joback Method
hvap	67.03	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	4.944		Crippen Method
mcvol	219.160	ml/mol	McGowan Method
pc	1656.49	kPa	Joback Method
rinpol	1944.00		NIST Webbook
rinpol	1944.00		NIST Webbook
tb	744.24	K	Joback Method
tc	938.48	K	Joback Method
tf	484.42	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	605.46	J/mol×K	744.24	Joback Method
cpg	618.07	J/mol×K	776.61	Joback Method
cpg	629.89	J/mol×K	808.99	Joback Method
cpg	640.91	J/mol×K	841.36	Joback Method
cpg	651.16	J/mol×K	873.73	Joback Method
cpg	660.65	J/mol×K	906.11	Joback Method
cpg	669.39	J/mol×K	938.48	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=U354164&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