4-Butylbenzoic acid, 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C16H16F8O2/c1-2-3-4-10-5-7-11(8-6-10)12(25)26-9-14(19,20)16(23,24)15(21

InchiKey: LYIBRZAOIWKJFF-UHFFFAOYSA-N

Formula: C16H16F8O2

SMILES: CCCCc1ccc(C(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)cc1

Mol. weight [g/mol]: 392.28

Physical Properties

Property code	Value	Unit	Source
gf	-1599.70	kJ/mol	Joback Method
hf	-1993.72	kJ/mol	Joback Method
hfus	32.51	kJ/mol	Joback Method
hvap	52.49	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	5.357		Crippen Method
mcvol	234.140	ml/mol	McGowan Method
pc	1385.05	kPa	Joback Method
rinpol	1725.00		NIST Webbook
tb	657.46	K	Joback Method
tc	828.12	K	Joback Method
tf	378.16	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.77	J/mol×K	657.46	Joback Method
cpg	685.79	J/mol×K	685.90	Joback Method
cpg	698.91	J/mol×K	714.35	Joback Method
cpg	711.18	J/mol×K	742.79	Joback Method
cpg	722.66	J/mol×K	771.24	Joback Method
cpg	733.38	J/mol×K	799.68	Joback Method
cpg	743.42	J/mol×K	828.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354161&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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