Phthalic acid, butyl 2,2,3,3,4,4,4-heptafluorobutyl ester

Inchi: InChI=1S/C16H15F7O4/c1-2-3-8-26-12(24)10-6-4-5-7-11(10)13(25)27-9-14(17,18)15(19

InchiKey: LAQIHCCHSQNFDR-UHFFFAOYSA-N

Formula: C16H15F7O4

SMILES: CCCCOC(=O)c1ccccc1C(=O)OCC(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 404.28

Physical Properties

Property code	Value	Unit	Source
gf	-1636.37	kJ/mol	Joback Method
hf	-2037.13	kJ/mol	Joback Method
hfus	35.74	kJ/mol	Joback Method
hvap	62.85	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.633		Crippen Method
mcvol	239.810	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	1794.00		NIST Webbook
rinpol	1794.00		NIST Webbook
tb	734.92	K	Joback Method
tc	917.01	K	Joback Method
tf	464.73	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.56	J/mol×K	734.92	Joback Method
cpg	721.96	J/mol×K	765.27	Joback Method
cpg	733.49	J/mol×K	795.62	Joback Method
cpg	744.19	J/mol×K	825.97	Joback Method
cpg	754.12	J/mol×K	856.31	Joback Method
cpg	763.32	J/mol×K	886.66	Joback Method
cpg	771.85	J/mol×K	917.01	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=U415542&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