Phthalic acid, ethyl 4-fluorobenzyl ester

Inchi: InChI=1S/C17H15FO4/c1-2-21-16(19)14-5-3-4-6-15(14)17(20)22-11-12-7-9-13(18)10-8-1
InchiKey: WOVFTHQUSHTQRG-UHFFFAOYSA-N
Formula: C17H15FO4
SMILES: CCOC(=O)c1ccccc1C(=O)OCc1ccc(F)cc1
Mol. weight [g/mol]: 302.30

Physical Properties

Property code	Value	Unit	Source
gf	-364.83	kJ/mol	Joback Method
hf	-629.80	kJ/mol	Joback Method
hfus	35.74	kJ/mol	Joback Method
hvap	76.81	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	3.359		Crippen Method
mcvol	219.520	ml/mol	McGowan Method
pc	2121.68	kPa	Joback Method
rinpol	2145.00		NIST Webbook
tb	803.53	K	Joback Method
tc	1027.80	K	Joback Method
tf	504.14	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.17	J/mol×K	803.53	Joback Method
cpg	632.24	J/mol×K	840.91	Joback Method
cpg	644.17	J/mol×K	878.29	Joback Method
cpg	654.97	J/mol×K	915.66	Joback Method
cpg	664.68	J/mol×K	953.04	Joback Method
cpg	673.31	J/mol×K	990.42	Joback Method
cpg	680.88	J/mol×K	1027.80	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377740&Units=SI

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