Phthalic acid, ethyl 3,4,5-trifluorobenzyl ester

Inchi: InChI=1S/C17H13F3O4/c1-2-23-16(21)11-5-3-4-6-12(11)17(22)24-9-10-7-13(18)15(20)1
InchiKey: CSFLUSMOSQADCE-UHFFFAOYSA-N
Formula: C17H13F3O4
SMILES: CCOC(=O)c1ccccc1C(=O)OCc1cc(F)c(F)c(F)c1
Mol. weight [g/mol]: 338.28

Physical Properties

Property code	Value	Unit	Source
gf	-773.71	kJ/mol	Joback Method
hf	-1044.96	kJ/mol	Joback Method
hfus	41.13	kJ/mol	Joback Method
hvap	76.50	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	3.638		Crippen Method
mcvol	223.060	ml/mol	McGowan Method
pc	1905.24	kPa	Joback Method
rinpol	2640.00		NIST Webbook
rinpol	2640.00		NIST Webbook
tb	812.03	K	Joback Method
tc	1023.37	K	Joback Method
tf	530.36	K	Joback Method
vc	0.874	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.67	J/mol×K	812.03	Joback Method
cpg	643.52	J/mol×K	847.25	Joback Method
cpg	654.37	J/mol×K	882.48	Joback Method
cpg	664.23	J/mol×K	917.70	Joback Method
cpg	673.09	J/mol×K	952.92	Joback Method
cpg	680.98	J/mol×K	988.14	Joback Method
cpg	687.89	J/mol×K	1023.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415474&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