Phthalic acid, ethyl 2,2,2-trifluoro-1-phenylethyl ester

Inchi: InChI=1S/C18H15F3O4/c1-2-24-16(22)13-10-6-7-11-14(13)17(23)25-15(18(19,20)21)12-
InchiKey: RGQLZDRUVMBJKU-UHFFFAOYSA-N
Formula: C18H15F3O4
SMILES: CCOC(=O)c1ccccc1C(=O)OC(c1ccccc1)C(F)(F)F
Mol. weight [g/mol]: 352.30

Physical Properties

Property code	Value	Unit	Source
gf	-736.00	kJ/mol	Joback Method
hf	-1045.22	kJ/mol	Joback Method
hfus	33.95	kJ/mol	Joback Method
hvap	75.05	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	4.324		Crippen Method
mcvol	237.150	ml/mol	McGowan Method
pc	1865.94	kPa	Joback Method
rinpol	2002.00		NIST Webbook
rinpol	2002.00		NIST Webbook
tb	816.30	K	Joback Method
tc	1034.62	K	Joback Method
tf	491.49	K	Joback Method
vc	0.912	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.03	J/mol×K	816.30	Joback Method
cpg	705.75	J/mol×K	852.69	Joback Method
cpg	717.32	J/mol×K	889.07	Joback Method
cpg	727.81	J/mol×K	925.46	Joback Method
cpg	737.26	J/mol×K	961.85	Joback Method
cpg	745.74	J/mol×K	998.23	Joback Method
cpg	753.30	J/mol×K	1034.62	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=U377699&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

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