Phthalic acid, propyl 4-trifluoromethoxybenzyl ester

Inchi: InChI=1S/C19H17F3O5/c1-2-11-25-17(23)15-5-3-4-6-16(15)18(24)26-12-13-7-9-14(10-8

InchiKey: BRJBLEICJRCEIZ-UHFFFAOYSA-N

Formula: C19H17F3O5

SMILES: CCCOC(=O)c1ccccc1C(=O)OCc1ccc(OC(F)(F)F)cc1

Mol. weight [g/mol]: 382.33

Physical Properties

Property code	Value	Unit	Source
gf	-839.77	kJ/mol	Joback Method
hf	-1204.27	kJ/mol	Joback Method
hfus	40.86	kJ/mol	Joback Method
hvap	80.74	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	4.509		Crippen Method
mcvol	257.110	ml/mol	McGowan Method
pc	1664.61	kPa	Joback Method
rinpol	2176.00		NIST Webbook
rinpol	2176.00		NIST Webbook
tb	867.02	K	Joback Method
tc	1081.34	K	Joback Method
tf	552.51	K	Joback Method
vc	0.993	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	773.36	J/mol×K	867.02	Joback Method
cpg	785.48	J/mol×K	902.74	Joback Method
cpg	796.42	J/mol×K	938.46	Joback Method
cpg	806.24	J/mol×K	974.18	Joback Method
cpg	814.95	J/mol×K	1009.90	Joback Method
cpg	822.60	J/mol×K	1045.62	Joback Method
cpg	829.21	J/mol×K	1081.34	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=U377684&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