Phthalic acid, 2,5-difluorobenzyl isobutyl ester

Inchi: InChI=1S/C19H18F2O4/c1-12(2)10-24-18(22)15-5-3-4-6-16(15)19(23)25-11-13-9-14(20)
InchiKey: CZSBLLVQSBAMPA-UHFFFAOYSA-N
Formula: C19H18F2O4
SMILES: CC(C)COC(=O)c1ccccc1C(=O)OCc1cc(F)ccc1F
Mol. weight [g/mol]: 348.34

Physical Properties

Property code	Value	Unit	Source
gf	-554.87	kJ/mol	Joback Method
hf	-883.94	kJ/mol	Joback Method
hfus	40.09	kJ/mol	Joback Method
hvap	80.72	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	4.135		Crippen Method
mcvol	249.470	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	2199.00		NIST Webbook
rinpol	2199.00		NIST Webbook
tb	853.10	K	Joback Method
tc	1069.89	K	Joback Method
tf	524.79	K	Joback Method
vc	0.962	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.42	J/mol×K	853.10	Joback Method
cpg	750.43	J/mol×K	889.23	Joback Method
cpg	762.27	J/mol×K	925.36	Joback Method
cpg	772.96	J/mol×K	961.49	Joback Method
cpg	782.51	J/mol×K	997.62	Joback Method
cpg	790.96	J/mol×K	1033.76	Joback Method
cpg	798.31	J/mol×K	1069.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377802&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