Phthalic acid, 2,5-difluorobenzyl pentyl ester

Inchi: InChI=1S/C20H20F2O4/c1-2-3-6-11-25-19(23)16-7-4-5-8-17(16)20(24)26-13-14-12-15(2
InchiKey: NGHHIPDRCYRXQZ-UHFFFAOYSA-N
Formula: C20H20F2O4
SMILES: CCCCCOC(=O)c1ccccc1C(=O)OCc1cc(F)ccc1F
Mol. weight [g/mol]: 362.37

Physical Properties

Property code	Value	Unit	Source
gf	-544.01	kJ/mol	Joback Method
hf	-899.30	kJ/mol	Joback Method
hfus	46.20	kJ/mol	Joback Method
hvap	83.33	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	4.669		Crippen Method
mcvol	263.560	ml/mol	McGowan Method
pc	1575.95	kPa	Joback Method
rinpol	2336.00		NIST Webbook
tb	876.42	K	Joback Method
tc	1090.09	K	Joback Method
tf	551.06	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.82	J/mol×K	876.42	Joback Method
cpg	806.87	J/mol×K	912.03	Joback Method
cpg	818.76	J/mol×K	947.64	Joback Method
cpg	829.50	J/mol×K	983.25	Joback Method
cpg	839.11	J/mol×K	1018.86	Joback Method
cpg	847.62	J/mol×K	1054.47	Joback Method
cpg	855.05	J/mol×K	1090.09	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=U377803&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