Phthalic acid, 2,5-difluorobenzyl octyl ester

Inchi: InChI=1S/C23H26F2O4/c1-2-3-4-5-6-9-14-28-22(26)19-10-7-8-11-20(19)23(27)29-16-17
InchiKey: PSAZRJHLEVHEQF-UHFFFAOYSA-N
Formula: C23H26F2O4
SMILES: CCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cc(F)ccc1F
Mol. weight [g/mol]: 404.45

Physical Properties

Property code	Value	Unit	Source
gf	-518.75	kJ/mol	Joback Method
hf	-961.22	kJ/mol	Joback Method
hfus	53.97	kJ/mol	Joback Method
hvap	90.01	kJ/mol	Joback Method
log10ws	-7.66		Crippen Method
logp	5.839		Crippen Method
mcvol	305.830	ml/mol	McGowan Method
pc	1269.16	kPa	Joback Method
rinpol	2639.00		NIST Webbook
rinpol	2639.00		NIST Webbook
tb	945.06	K	Joback Method
tc	1161.56	K	Joback Method
tf	584.87	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	968.92	J/mol×K	945.06	Joback Method
cpg	982.41	J/mol×K	981.14	Joback Method
cpg	994.58	J/mol×K	1017.23	Joback Method
cpg	1005.48	J/mol×K	1053.31	Joback Method
cpg	1015.14	J/mol×K	1089.39	Joback Method
cpg	1023.60	J/mol×K	1125.48	Joback Method
cpg	1030.89	J/mol×K	1161.56	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=U377805&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