Phthalic acid, octyl 4-trifluoromethoxybenzyl ester

Inchi: InChI=1S/C24H27F3O5/c1-2-3-4-5-6-9-16-30-22(28)20-10-7-8-11-21(20)23(29)31-17-18
InchiKey: NGDMSOPDFDTKPR-UHFFFAOYSA-N
Formula: C24H27F3O5
SMILES: CCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccc(OC(F)(F)F)cc1
Mol. weight [g/mol]: 452.46

Physical Properties

Property code	Value	Unit	Source
gf	-797.67	kJ/mol	Joback Method
hf	-1307.47	kJ/mol	Joback Method
hfus	53.81	kJ/mol	Joback Method
hvap	91.87	kJ/mol	Joback Method
log10ws	-8.27		Crippen Method
logp	6.460		Crippen Method
mcvol	327.560	ml/mol	McGowan Method
pc	1164.04	kPa	Joback Method
rinpol	2678.00		NIST Webbook
rinpol	2678.00		NIST Webbook
tb	981.42	K	Joback Method
tc	1202.69	K	Joback Method
tf	608.86	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1063.98	J/mol×K	981.42	Joback Method
cpg	1076.77	J/mol×K	1018.30	Joback Method
cpg	1088.19	J/mol×K	1055.18	Joback Method
cpg	1098.28	J/mol×K	1092.05	Joback Method
cpg	1107.12	J/mol×K	1128.93	Joback Method
cpg	1114.74	J/mol×K	1165.81	Joback Method
cpg	1121.20	J/mol×K	1202.69	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=U377690&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