Phthalic acid, pentadecyl 4-trifluoromethoxybenzyl ester

Inchi: InChI=1S/C31H41F3O5/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-23-37-29(35)27-17-14-15-18

InchiKey: XVNIQYXDLPXEML-UHFFFAOYSA-N

Formula: C31H41F3O5

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

Mol. weight [g/mol]: 550.65

Physical Properties

Property code	Value	Unit	Source
gf	-738.73	kJ/mol	Joback Method
hf	-1451.95	kJ/mol	Joback Method
hfus	71.94	kJ/mol	Joback Method
hvap	107.45	kJ/mol	Joback Method
log10ws	-11.20		Crippen Method
logp	9.190		Crippen Method
mcvol	426.190	ml/mol	McGowan Method
pc	770.32	kPa	Joback Method
rinpol	3288.00		NIST Webbook
rinpol	3288.00		NIST Webbook
tb	1141.58	K	Joback Method
tc	1416.48	K	Joback Method
tf	687.75	K	Joback Method
vc	1.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1490.32	J/mol×K	1141.58	Joback Method
cpg	1504.48	J/mol×K	1187.40	Joback Method
cpg	1516.55	J/mol×K	1233.21	Joback Method
cpg	1526.68	J/mol×K	1279.03	Joback Method
cpg	1535.04	J/mol×K	1324.85	Joback Method
cpg	1541.77	J/mol×K	1370.66	Joback Method
cpg	1547.02	J/mol×K	1416.48	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=U377696&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