Phthalic acid, hexadecyl 4-trifluoromethoxybenzyl ester

Inchi: InChI=1S/C32H43F3O5/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-24-38-30(36)28-18-15-16

InchiKey: HIJNNZIMYJBWFF-UHFFFAOYSA-N

Formula: C32H43F3O5

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

Mol. weight [g/mol]: 564.68

Physical Properties

Property code	Value	Unit	Source
gf	-730.31	kJ/mol	Joback Method
hf	-1472.59	kJ/mol	Joback Method
hfus	74.53	kJ/mol	Joback Method
hvap	109.68	kJ/mol	Joback Method
log10ws	-11.62		Crippen Method
logp	9.580		Crippen Method
mcvol	440.280	ml/mol	McGowan Method
pc	730.86	kPa	Joback Method
rinpol	3387.00		NIST Webbook
rinpol	3387.00		NIST Webbook
tb	1164.46	K	Joback Method
tc	1452.62	K	Joback Method
tf	699.02	K	Joback Method
vc	1.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1552.40	J/mol×K	1164.46	Joback Method
cpg	1566.85	J/mol×K	1212.49	Joback Method
cpg	1579.05	J/mol×K	1260.51	Joback Method
cpg	1589.18	J/mol×K	1308.54	Joback Method
cpg	1597.42	J/mol×K	1356.57	Joback Method
cpg	1603.97	J/mol×K	1404.59	Joback Method
cpg	1609.00	J/mol×K	1452.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377697&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

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