Phthalic acid, nonyl 4-trifluoromethoxybenzyl ester

Inchi: InChI=1S/C25H29F3O5/c1-2-3-4-5-6-7-10-17-31-23(29)21-11-8-9-12-22(21)24(30)32-18

InchiKey: PZQNPQLQYQBDAZ-UHFFFAOYSA-N

Formula: C25H29F3O5

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

Mol. weight [g/mol]: 466.49

Physical Properties

Property code	Value	Unit	Source
gf	-789.25	kJ/mol	Joback Method
hf	-1328.11	kJ/mol	Joback Method
hfus	56.40	kJ/mol	Joback Method
hvap	94.09	kJ/mol	Joback Method
log10ws	-8.69		Crippen Method
logp	6.850		Crippen Method
mcvol	341.650	ml/mol	McGowan Method
pc	1091.38	kPa	Joback Method
rinpol	2781.00		NIST Webbook
tb	1004.30	K	Joback Method
tc	1229.67	K	Joback Method
tf	620.13	K	Joback Method
vc	1.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1123.76	J/mol×K	1004.30	Joback Method
cpg	1136.70	J/mol×K	1041.86	Joback Method
cpg	1148.19	J/mol×K	1079.42	Joback Method
cpg	1158.31	J/mol×K	1116.98	Joback Method
cpg	1167.11	J/mol×K	1154.55	Joback Method
cpg	1174.66	J/mol×K	1192.11	Joback Method
cpg	1181.01	J/mol×K	1229.67	Joback Method

Sources

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=U377691&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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