Phthalic acid, undecyl 2-trifluoromethylbenzyl ester

Other names: Phthalic acid, 2-trifluorobenzyl undecyl ester
Inchi: InChI=1S/C27H33F3O4/c1-2-3-4-5-6-7-8-9-14-19-33-25(31)22-16-11-12-17-23(22)26(32
InchiKey: QIZDENQBWLXPIO-UHFFFAOYSA-N
Formula: C27H33F3O4
SMILES: CCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccccc1C(F)(F)F
Mol. weight [g/mol]: 478.54

Physical Properties

Property code	Value	Unit	Source
gf	-667.41	kJ/mol	Joback Method
hf	-1237.17	kJ/mol	Joback Method
hfus	60.39	kJ/mol	Joback Method
hvap	96.14	kJ/mol	Joback Method
log10ws	-9.36		Crippen Method
logp	7.750		Crippen Method
mcvol	363.960	ml/mol	McGowan Method
pc	975.34	kPa	Joback Method
rinpol	3009.00		NIST Webbook
rinpol	3009.00		NIST Webbook
tb	1027.64	K	Joback Method
tc	1258.34	K	Joback Method
tf	620.44	K	Joback Method
vc	1.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1218.03	J/mol×K	1027.64	Joback Method
cpg	1232.31	J/mol×K	1066.09	Joback Method
cpg	1245.21	J/mol×K	1104.54	Joback Method
cpg	1256.84	J/mol×K	1142.99	Joback Method
cpg	1267.28	J/mol×K	1181.44	Joback Method
cpg	1276.62	J/mol×K	1219.89	Joback Method
cpg	1284.97	J/mol×K	1258.34	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=U377826&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