Phthalic acid, dodecyl 2-trifluoromethylbenzyl ester

Other names: Phthalic acid, dodecyl 2-trifluorobenzyl ester
Inchi: InChI=1S/C28H35F3O4/c1-2-3-4-5-6-7-8-9-10-15-20-34-26(32)23-17-12-13-18-24(23)27
InchiKey: NMNXREAAKZBSGU-UHFFFAOYSA-N
Formula: C28H35F3O4
SMILES: CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccccc1C(F)(F)F
Mol. weight [g/mol]: 492.57

Physical Properties

Property code	Value	Unit	Source
gf	-658.99	kJ/mol	Joback Method
hf	-1257.81	kJ/mol	Joback Method
hfus	62.98	kJ/mol	Joback Method
hvap	98.36	kJ/mol	Joback Method
log10ws	-9.77		Crippen Method
logp	8.140		Crippen Method
mcvol	378.050	ml/mol	McGowan Method
pc	919.39	kPa	Joback Method
rinpol	3111.00		NIST Webbook
rinpol	3111.00		NIST Webbook
tb	1050.52	K	Joback Method
tc	1287.63	K	Joback Method
tf	631.71	K	Joback Method
vc	1.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1279.35	J/mol×K	1050.52	Joback Method
cpg	1293.92	J/mol×K	1090.04	Joback Method
cpg	1307.06	J/mol×K	1129.56	Joback Method
cpg	1318.86	J/mol×K	1169.07	Joback Method
cpg	1329.44	J/mol×K	1208.59	Joback Method
cpg	1338.90	J/mol×K	1248.11	Joback Method
cpg	1347.34	J/mol×K	1287.63	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=U377827&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