Phthalic acid, dodecyl 2,2,2-trifluoro-1-phenylethyl ester

Inchi: InChI=1S/C28H35F3O4/c1-2-3-4-5-6-7-8-9-10-16-21-34-26(32)23-19-14-15-20-24(23)27

InchiKey: ZMHZBZSWWPQXEK-UHFFFAOYSA-N

Formula: C28H35F3O4

SMILES: CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OC(c1ccccc1)C(F)(F)F

Mol. weight [g/mol]: 492.57

Physical Properties

Property code	Value	Unit	Source
gf	-651.80	kJ/mol	Joback Method
hf	-1251.62	kJ/mol	Joback Method
hfus	59.85	kJ/mol	Joback Method
hvap	97.31	kJ/mol	Joback Method
log10ws	-9.72		Crippen Method
logp	8.225		Crippen Method
mcvol	378.050	ml/mol	McGowan Method
pc	932.35	kPa	Joback Method
rinpol	2999.00		NIST Webbook
rinpol	2999.00		NIST Webbook
tb	1045.10	K	Joback Method
tc	1280.27	K	Joback Method
tf	604.19	K	Joback Method
vc	1.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1280.74	J/mol×K	1045.10	Joback Method
cpg	1295.35	J/mol×K	1084.29	Joback Method
cpg	1308.57	J/mol×K	1123.49	Joback Method
cpg	1320.49	J/mol×K	1162.68	Joback Method
cpg	1331.24	J/mol×K	1201.88	Joback Method
cpg	1340.93	J/mol×K	1241.07	Joback Method
cpg	1349.66	J/mol×K	1280.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377710&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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