Terephthalic acid, octyl 2,2,2-trifluoro-1-phenylethyl ester

Inchi: InChI=1S/C24H27F3O4/c1-2-3-4-5-6-10-17-30-22(28)19-13-15-20(16-14-19)23(29)31-21

InchiKey: BUTFKYREQLJFKU-UHFFFAOYSA-N

Formula: C24H27F3O4

SMILES: CCCCCCCCOC(=O)c1ccc(C(=O)OC(c2ccccc2)C(F)(F)F)cc1

Mol. weight [g/mol]: 436.46

Physical Properties

Property code	Value	Unit	Source
gf	-685.48	kJ/mol	Joback Method
hf	-1169.06	kJ/mol	Joback Method
hfus	49.49	kJ/mol	Joback Method
hvap	88.41	kJ/mol	Joback Method
log10ws	-8.04		Crippen Method
logp	6.664		Crippen Method
mcvol	321.690	ml/mol	McGowan Method
pc	1196.48	kPa	Joback Method
rinpol	2534.00		NIST Webbook
rinpol	2534.00		NIST Webbook
tb	953.58	K	Joback Method
tc	1171.54	K	Joback Method
tf	559.11	K	Joback Method
vc	1.248	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1038.40	J/mol×K	953.58	Joback Method
cpg	1052.09	J/mol×K	989.91	Joback Method
cpg	1064.56	J/mol×K	1026.23	Joback Method
cpg	1075.86	J/mol×K	1062.56	Joback Method
cpg	1086.09	J/mol×K	1098.89	Joback Method
cpg	1095.31	J/mol×K	1135.21	Joback Method
cpg	1103.59	J/mol×K	1171.54	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415989&Units=SI

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

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