Terephthalic acid, decyl 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C21H29F3O4/c1-3-4-5-6-7-8-9-10-15-27-19(25)17-11-13-18(14-12-17)20(26)2

InchiKey: RNPGLGWAIWZWRL-UHFFFAOYSA-N

Formula: C21H29F3O4

SMILES: CCCCCCCCCCOC(=O)c1ccc(C(=O)OC(C)C(F)(F)F)cc1

Mol. weight [g/mol]: 402.45

Physical Properties

Property code	Value	Unit	Source
gf	-823.15	kJ/mol	Joback Method
hf	-1343.67	kJ/mol	Joback Method
hfus	47.67	kJ/mol	Joback Method
hvap	79.45	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	6.092		Crippen Method
mcvol	303.180	ml/mol	McGowan Method
pc	1161.66	kPa	Joback Method
rinpol	2536.00		NIST Webbook
rinpol	2536.00		NIST Webbook
tb	858.26	K	Joback Method
tc	1054.92	K	Joback Method
tf	498.88	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	960.32	J/mol×K	858.26	Joback Method
cpg	975.77	J/mol×K	891.04	Joback Method
cpg	990.11	J/mol×K	923.81	Joback Method
cpg	1003.40	J/mol×K	956.59	Joback Method
cpg	1015.66	J/mol×K	989.37	Joback Method
cpg	1026.95	J/mol×K	1022.14	Joback Method
cpg	1037.30	J/mol×K	1054.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415769&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

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