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

Inchi: InChI=1S/C19H25F3O4/c1-3-4-5-6-7-8-13-25-17(23)15-9-11-16(12-10-15)18(24)26-14(2

InchiKey: BZMALCXOVULWCD-UHFFFAOYSA-N

Formula: C19H25F3O4

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

Mol. weight [g/mol]: 374.39

Physical Properties

Property code	Value	Unit	Source
gf	-839.99	kJ/mol	Joback Method
hf	-1302.39	kJ/mol	Joback Method
hfus	42.49	kJ/mol	Joback Method
hvap	75.00	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	5.312		Crippen Method
mcvol	275.000	ml/mol	McGowan Method
pc	1330.04	kPa	Joback Method
rinpol	2340.00		NIST Webbook
rinpol	2340.00		NIST Webbook
tb	812.50	K	Joback Method
tc	1005.75	K	Joback Method
tf	476.34	K	Joback Method
vc	1.077	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.33	J/mol×K	812.50	Joback Method
cpg	858.21	J/mol×K	844.71	Joback Method
cpg	872.07	J/mol×K	876.92	Joback Method
cpg	884.94	J/mol×K	909.12	Joback Method
cpg	896.86	J/mol×K	941.33	Joback Method
cpg	907.87	J/mol×K	973.54	Joback Method
cpg	917.99	J/mol×K	1005.75	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=U415767&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