Terephthalic acid, decyl 2,2,2-trifluoroethyl ester

Inchi: InChI=1S/C20H27F3O4/c1-2-3-4-5-6-7-8-9-14-26-18(24)16-10-12-17(13-11-16)19(25)27
InchiKey: KWBQMTHFJVMENH-UHFFFAOYSA-N
Formula: C20H27F3O4
SMILES: CCCCCCCCCCOC(=O)c1ccc(C(=O)OCC(F)(F)F)cc1
Mol. weight [g/mol]: 388.42

Physical Properties

Property code	Value	Unit	Source
gf	-829.13	kJ/mol	Joback Method
hf	-1317.75	kJ/mol	Joback Method
hfus	48.61	kJ/mol	Joback Method
hvap	77.62	kJ/mol	Joback Method
log10ws	-6.81		Crippen Method
logp	5.703		Crippen Method
mcvol	289.090	ml/mol	McGowan Method
pc	1234.61	kPa	Joback Method
rinpol	2537.00		NIST Webbook
rinpol	2537.00		NIST Webbook
tb	835.82	K	Joback Method
tc	1029.17	K	Joback Method
tf	502.61	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	900.91	J/mol×K	835.82	Joback Method
cpg	915.99	J/mol×K	868.05	Joback Method
cpg	930.02	J/mol×K	900.27	Joback Method
cpg	943.06	J/mol×K	932.50	Joback Method
cpg	955.14	J/mol×K	964.72	Joback Method
cpg	966.29	J/mol×K	996.95	Joback Method
cpg	976.56	J/mol×K	1029.17	Joback Method

Sources

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=U383045&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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