Terephthalic acid, heptyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C21H21F3O4/c1-2-3-4-5-6-13-27-20(25)14-7-9-15(10-8-14)21(26)28-17-12-11

InchiKey: UKRBTEFKYUUSFY-UHFFFAOYSA-N

Formula: C21H21F3O4

SMILES: CCCCCCCOC(=O)c1ccc(C(=O)Oc2ccc(F)c(F)c2F)cc1

Mol. weight [g/mol]: 394.38

Physical Properties

Property code	Value	Unit	Source
gf	-740.03	kJ/mol	Joback Method
hf	-1127.52	kJ/mol	Joback Method
hfus	51.49	kJ/mol	Joback Method
hvap	85.40	kJ/mol	Joback Method
log10ws	-7.31		Crippen Method
logp	5.450		Crippen Method
mcvol	279.420	ml/mol	McGowan Method
pc	1397.50	kPa	Joback Method
rinpol	2830.00		NIST Webbook
rinpol	2830.00		NIST Webbook
tb	903.55	K	Joback Method
tc	1114.31	K	Joback Method
tf	575.44	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	857.56	J/mol×K	903.55	Joback Method
cpg	870.32	J/mol×K	938.68	Joback Method
cpg	881.90	J/mol×K	973.80	Joback Method
cpg	892.31	J/mol×K	1008.93	Joback Method
cpg	901.59	J/mol×K	1044.06	Joback Method
cpg	909.74	J/mol×K	1079.18	Joback Method
cpg	916.79	J/mol×K	1114.31	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=U415803&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