Sebacic acid, di(3,5-difluorophenyl) ester

Inchi: InChI=1S/C22H22F4O4/c23-15-9-16(24)12-19(11-15)29-21(27)7-5-3-1-2-4-6-8-22(28)30
InchiKey: RWIJULKZYJEZNK-UHFFFAOYSA-N
Formula: C22H22F4O4
SMILES: O=C(CCCCCCCCC(=O)Oc1cc(F)cc(F)c1)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]: 426.40

Physical Properties

Property code	Value	Unit	Source
gf	-926.42	kJ/mol	Joback Method
hf	-1344.27	kJ/mol	Joback Method
hfus	57.16	kJ/mol	Joback Method
hvap	86.81	kJ/mol	Joback Method
log10ws	-7.59		Crippen Method
logp	5.875		Crippen Method
mcvol	295.280	ml/mol	McGowan Method
pc	1261.06	kPa	Joback Method
rinpol	2712.00		NIST Webbook
tb	925.70	K	Joback Method
tc	1135.80	K	Joback Method
tf	587.30	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	922.99	J/mol×K	925.70	Joback Method
cpg	935.66	J/mol×K	960.72	Joback Method
cpg	947.12	J/mol×K	995.73	Joback Method
cpg	957.40	J/mol×K	1030.75	Joback Method
cpg	966.51	J/mol×K	1065.77	Joback Method
cpg	974.48	J/mol×K	1100.79	Joback Method
cpg	981.33	J/mol×K	1135.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354541&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