Sebacic acid, di(2-(2-fluorophenyl)ethyl) ester

Inchi: InChI=1S/C26H32F2O4/c27-23-13-9-7-11-21(23)17-19-31-25(29)15-5-3-1-2-4-6-16-26(3
InchiKey: QPMKHKCKZHIWJP-UHFFFAOYSA-N
Formula: C26H32F2O4
SMILES: O=C(CCCCCCCCC(=O)OCCc1ccccc1F)OCCc1ccccc1F
Mol. weight [g/mol]: 446.53

Physical Properties

Property code	Value	Unit	Source
gf	-483.86	kJ/mol	Joback Method
hf	-1011.67	kJ/mol	Joback Method
hfus	62.13	kJ/mol	Joback Method
hvap	96.02	kJ/mol	Joback Method
log10ws	-7.30		Crippen Method
logp	5.957		Crippen Method
mcvol	348.100	ml/mol	McGowan Method
pc	1054.14	kPa	Joback Method
rinpol	3136.00		NIST Webbook
rinpol	3136.00		NIST Webbook
tb	1008.72	K	Joback Method
tc	1234.96	K	Joback Method
tf	606.16	K	Joback Method
vc	1.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1150.21	J/mol×K	1008.72	Joback Method
cpg	1164.27	J/mol×K	1046.43	Joback Method
cpg	1176.85	J/mol×K	1084.13	Joback Method
cpg	1188.02	J/mol×K	1121.84	Joback Method
cpg	1197.84	J/mol×K	1159.55	Joback Method
cpg	1206.36	J/mol×K	1197.25	Joback Method
cpg	1213.64	J/mol×K	1234.96	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=U380747&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