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

Inchi: InChI=1S/C21H31FO4/c1-2-16-25-20(23)13-7-5-3-4-6-8-14-21(24)26-17-15-18-11-9-10-1

InchiKey: GZIMVAVNYGXMQO-UHFFFAOYSA-N

Formula: C21H31FO4

SMILES: CCCOC(=O)CCCCCCCCC(=O)OCCc1ccccc1F

Mol. weight [g/mol]: 366.47

Physical Properties

Property code	Value	Unit	Source
gf	-433.93	kJ/mol	Joback Method
hf	-937.42	kJ/mol	Joback Method
hfus	52.45	kJ/mol	Joback Method
hvap	82.77	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	4.985		Crippen Method
mcvol	299.640	ml/mol	McGowan Method
pc	1213.20	kPa	Joback Method
rinpol	2565.00		NIST Webbook
rinpol	2565.00		NIST Webbook
tb	863.39	K	Joback Method
tc	1061.63	K	Joback Method
tf	510.28	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	944.43	J/mol×K	863.39	Joback Method
cpg	960.43	J/mol×K	896.43	Joback Method
cpg	975.28	J/mol×K	929.47	Joback Method
cpg	989.02	J/mol×K	962.51	Joback Method
cpg	1001.66	J/mol×K	995.55	Joback Method
cpg	1013.24	J/mol×K	1028.59	Joback Method
cpg	1023.76	J/mol×K	1061.63	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=U380743&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