Sebacic acid, 1-(4-fluorophenyl)ethyl hexyl ester

Inchi: InChI=1S/C24H37FO4/c1-3-4-5-12-19-28-23(26)13-10-8-6-7-9-11-14-24(27)29-20(2)21-1

InchiKey: ZBRMVSOUWSLIKM-UHFFFAOYSA-N

Formula: C24H37FO4

SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)OC(C)c1ccc(F)cc1

Mol. weight [g/mol]: 408.55

Physical Properties

Property code	Value	Unit	Source
gf	-411.11	kJ/mol	Joback Method
hf	-1004.62	kJ/mol	Joback Method
hfus	56.70	kJ/mol	Joback Method
hvap	89.06	kJ/mol	Joback Method
log10ws	-7.49		Crippen Method
logp	6.674		Crippen Method
mcvol	341.910	ml/mol	McGowan Method
pc	1007.17	kPa	Joback Method
rinpol	2759.00		NIST Webbook
rinpol	2759.00		NIST Webbook
tb	931.59	K	Joback Method
tc	1140.67	K	Joback Method
tf	529.09	K	Joback Method
vc	1.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1126.85	J/mol×K	931.59	Joback Method
cpg	1143.68	J/mol×K	966.44	Joback Method
cpg	1159.14	J/mol×K	1001.28	Joback Method
cpg	1173.26	J/mol×K	1036.13	Joback Method
cpg	1186.10	J/mol×K	1070.98	Joback Method
cpg	1197.67	J/mol×K	1105.82	Joback Method
cpg	1208.04	J/mol×K	1140.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380740&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

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