Sebacic acid, decyl 2-fluorophenyl ester

Inchi: InChI=1S/C26H41FO4/c1-2-3-4-5-6-9-12-17-22-30-25(28)20-13-10-7-8-11-14-21-26(29)3
InchiKey: QYENDWGXCVTGMF-UHFFFAOYSA-N
Formula: C26H41FO4
SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccccc1F
Mol. weight [g/mol]: 436.60

Physical Properties

Property code	Value	Unit	Source
gf	-391.83	kJ/mol	Joback Method
hf	-1040.62	kJ/mol	Joback Method
hfus	65.40	kJ/mol	Joback Method
hvap	93.90	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	7.536		Crippen Method
mcvol	370.090	ml/mol	McGowan Method
pc	890.54	kPa	Joback Method
rinpol	3109.00		NIST Webbook
rinpol	3109.00		NIST Webbook
tb	977.79	K	Joback Method
tc	1198.89	K	Joback Method
tf	566.63	K	Joback Method
vc	1.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1250.48	J/mol×K	977.79	Joback Method
cpg	1268.01	J/mol×K	1014.64	Joback Method
cpg	1283.99	J/mol×K	1051.49	Joback Method
cpg	1298.47	J/mol×K	1088.34	Joback Method
cpg	1311.49	J/mol×K	1125.19	Joback Method
cpg	1323.11	J/mol×K	1162.04	Joback Method
cpg	1333.39	J/mol×K	1198.89	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355004&Units=SI

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

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