

Sebacic acid, 3-fluorophenyl tridecyl ester

Inchi:	InChI=1S/C29H47FO4/c1-2-3-4-5-6-7-8-9-12-15-18-24-33-28(31)22-16-13-10-11-14-17-2
InchiKey:	JSCSFTCJGCLLEW-UHFFFAOYSA-N
Formula:	C29H47FO4
SMILES:	CCCCCCCCCCCCOC(=O)CCCCCCCC(=O)Oc1cccc(F)c1
Mol. weight [g/mol]:	478.68

Physical Properties

Property code	Value	Unit	Source
gf	-366.57	kJ/mol	Joback Method
hf	-1102.54	kJ/mol	Joback Method
hfus	73.17	kJ/mol	Joback Method
hvap	100.58	kJ/mol	Joback Method
log10ws	-9.77		Crippen Method
logp	8.706		Crippen Method
mvol	412.360	ml/mol	McGowan Method
pc	755.15	kPa	Joback Method
rinpol	3391.00		NIST Webbook
rinpol	3391.00		NIST Webbook
tb	1046.43	K	Joback Method
tc	1294.45	K	Joback Method
tf	600.44	K	Joback Method
vc	1.617	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1439.60	J/molxK	1046.43	Joback Method
cpg	1458.39	J/molxK	1087.77	Joback Method
cpg	1475.19	J/molxK	1129.10	Joback Method
cpg	1490.09	J/molxK	1170.44	Joback Method
cpg	1503.19	J/molxK	1211.78	Joback Method
cpg	1514.56	J/molxK	1253.11	Joback Method
cpg	1524.31	J/molxK	1294.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355019&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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