Succinic acid, di(4-fluorophenethyl) ester

Inchi: InChI=1S/C20H20F2O4/c21-17-5-1-15(2-6-17)11-13-25-19(23)9-10-20(24)26-14-12-16-3-7-18(22)8-4-16/h1-8H,9-14H2

InchiKey: UJZLPQFPMMBXCZ-UHFFFAOYSA-N

Formula: C20H20F2O4

SMILES: O=C(CCC(=O)OCCc1ccc(F)cc1)OCCc1ccc(F)cc1

Mol. weight [g/mol]: 362.37

Physical Properties

Property code	Value	Unit	Source
gf	-534.38	kJ/mol	Joback Method
hf	-887.83	kJ/mol	Joback Method
hfus	46.59	kJ/mol	Joback Method
hvap	82.67	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	3.617		Crippen Method
mcvol	263.560	ml/mol	McGowan Method
pc	1594.89	kPa	Joback Method
rinpol	2562.00		NIST Webbook
rinpol	2562.00		NIST Webbook
tb	871.44	K	Joback Method
tc	1084.29	K	Joback Method
tf	538.54	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.00	J/mol×K	871.44	Joback Method
cpg	808.15	J/mol×K	906.92	Joback Method
cpg	820.14	J/mol×K	942.39	Joback Method
cpg	830.99	J/mol×K	977.87	Joback Method
cpg	840.73	J/mol×K	1013.34	Joback Method
cpg	849.41	J/mol×K	1048.82	Joback Method
cpg	857.03	J/mol×K	1084.29	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=U381311&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