Sebacic acid, 3,5-difluorophenyl isobutyl ester

Inchi: InChI=1S/C20H28F2O4/c1-15(2)14-25-19(23)9-7-5-3-4-6-8-10-20(24)26-18-12-16(21)11
InchiKey: DBCSXXJYJFDXFL-UHFFFAOYSA-N
Formula: C20H28F2O4
SMILES: CC(C)COC(=O)CCCCCCCCC(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]: 370.43

Physical Properties

Property code	Value	Unit	Source
gf	-649.23	kJ/mol	Joback Method
hf	-1129.64	kJ/mol	Joback Method
hfus	49.03	kJ/mol	Joback Method
hvap	80.00	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	5.190		Crippen Method
mcvol	287.320	ml/mol	McGowan Method
pc	1251.26	kPa	Joback Method
rinpol	2399.00		NIST Webbook
rinpol	2399.00		NIST Webbook
tb	844.32	K	Joback Method
tc	1039.66	K	Joback Method
tf	497.12	K	Joback Method
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.31	J/mol×K	844.32	Joback Method
cpg	907.71	J/mol×K	876.88	Joback Method
cpg	922.02	J/mol×K	909.43	Joback Method
cpg	935.26	J/mol×K	941.99	Joback Method
cpg	947.45	J/mol×K	974.54	Joback Method
cpg	958.60	J/mol×K	1007.10	Joback Method
cpg	968.74	J/mol×K	1039.66	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=U354524&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