Sebacic acid, butyl 3,5-difluorophenyl ester

Inchi: InChI=1S/C20H28F2O4/c1-2-3-12-25-19(23)10-8-6-4-5-7-9-11-20(24)26-18-14-16(21)13
InchiKey: JKNVUVMBWHOJJT-UHFFFAOYSA-N
Formula: C20H28F2O4
SMILES: CCCCOC(=O)CCCCCCCCC(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]: 370.43

Physical Properties

Property code	Value	Unit	Source
gf	-646.79	kJ/mol	Joback Method
hf	-1124.36	kJ/mol	Joback Method
hfus	52.55	kJ/mol	Joback Method
hvap	80.39	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	5.334		Crippen Method
mcvol	287.320	ml/mol	McGowan Method
pc	1244.21	kPa	Joback Method
rinpol	2447.00		NIST Webbook
rinpol	2447.00		NIST Webbook
tb	844.76	K	Joback Method
tc	1038.99	K	Joback Method
tf	512.12	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	891.79	J/mol×K	844.76	Joback Method
cpg	907.11	J/mol×K	877.13	Joback Method
cpg	921.37	J/mol×K	909.50	Joback Method
cpg	934.58	J/mol×K	941.87	Joback Method
cpg	946.76	J/mol×K	974.24	Joback Method
cpg	957.92	J/mol×K	1006.62	Joback Method
cpg	968.09	J/mol×K	1038.99	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=U354525&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