Sebacic acid, butyl 3-fluorophenyl ester

Inchi: InChI=1S/C20H29FO4/c1-2-3-15-24-19(22)13-8-6-4-5-7-9-14-20(23)25-18-12-10-11-17(2
InchiKey: AVWNWVFXBAOTTM-UHFFFAOYSA-N
Formula: C20H29FO4
SMILES: CCCCOC(=O)CCCCCCCCC(=O)Oc1cccc(F)c1
Mol. weight [g/mol]: 352.44

Physical Properties

Property code	Value	Unit	Source
gf	-442.35	kJ/mol	Joback Method
hf	-916.78	kJ/mol	Joback Method
hfus	49.86	kJ/mol	Joback Method
hvap	80.55	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.195		Crippen Method
mcvol	285.550	ml/mol	McGowan Method
pc	1298.60	kPa	Joback Method
rinpol	2483.00		NIST Webbook
tb	840.51	K	Joback Method
tc	1036.82	K	Joback Method
tf	499.01	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.09	J/mol×K	840.51	Joback Method
cpg	900.82	J/mol×K	873.23	Joback Method
cpg	915.47	J/mol×K	905.95	Joback Method
cpg	929.04	J/mol×K	938.67	Joback Method
cpg	941.57	J/mol×K	971.38	Joback Method
cpg	953.08	J/mol×K	1004.10	Joback Method
cpg	963.58	J/mol×K	1036.82	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=U355011&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