Sebacic acid, 2,5-difluorobenzyl ethyl ester

Inchi: InChI=1S/C19H26F2O4/c1-2-24-18(22)9-7-5-3-4-6-8-10-19(23)25-14-15-13-16(20)11-12
InchiKey: KEMJYKIVYUUBNT-UHFFFAOYSA-N
Formula: C19H26F2O4
SMILES: CCOC(=O)CCCCCCCCC(=O)OCc1cc(F)ccc1F
Mol. weight [g/mol]: 356.40

Physical Properties

Property code	Value	Unit	Source
gf	-655.21	kJ/mol	Joback Method
hf	-1103.72	kJ/mol	Joback Method
hfus	49.96	kJ/mol	Joback Method
hvap	78.17	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.692		Crippen Method
mcvol	273.230	ml/mol	McGowan Method
pc	1332.96	kPa	Joback Method
rinpol	2335.00		NIST Webbook
rinpol	2335.00		NIST Webbook
tb	821.88	K	Joback Method
tc	1014.18	K	Joback Method
tf	500.85	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	833.28	J/mol×K	821.88	Joback Method
cpg	848.29	J/mol×K	853.93	Joback Method
cpg	862.28	J/mol×K	885.98	Joback Method
cpg	875.29	J/mol×K	918.03	Joback Method
cpg	887.31	J/mol×K	950.08	Joback Method
cpg	898.37	J/mol×K	982.13	Joback Method
cpg	908.49	J/mol×K	1014.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380760&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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