Sebacic acid, 2,5-difluorobenzyl isobutyl ester

Inchi: InChI=1S/C21H30F2O4/c1-16(2)14-26-20(24)9-7-5-3-4-6-8-10-21(25)27-15-17-13-18(22
InchiKey: JAQPDLZHJXAQPR-UHFFFAOYSA-N
Formula: C21H30F2O4
SMILES: CC(C)COC(=O)CCCCCCCCC(=O)OCc1cc(F)ccc1F
Mol. weight [g/mol]: 384.46

Physical Properties

Property code	Value	Unit	Source
gf	-640.81	kJ/mol	Joback Method
hf	-1150.28	kJ/mol	Joback Method
hfus	51.62	kJ/mol	Joback Method
hvap	82.23	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	5.328		Crippen Method
mcvol	301.410	ml/mol	McGowan Method
pc	1170.42	kPa	Joback Method
rinpol	2487.00		NIST Webbook
rinpol	2487.00		NIST Webbook
tb	867.20	K	Joback Method
tc	1064.90	K	Joback Method
tf	508.39	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	951.57	J/mol×K	867.20	Joback Method
cpg	967.26	J/mol×K	900.15	Joback Method
cpg	981.79	J/mol×K	933.10	Joback Method
cpg	995.20	J/mol×K	966.05	Joback Method
cpg	1007.49	J/mol×K	999.00	Joback Method
cpg	1018.71	J/mol×K	1031.95	Joback Method
cpg	1028.85	J/mol×K	1064.90	Joback Method

Sources

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=U380762&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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