Sebacic acid, di(2,5-difluorobenzyl) ester

Inchi: InChI=1S/C24H26F4O4/c25-19-9-11-21(27)17(13-19)15-31-23(29)7-5-3-1-2-4-6-8-24(30
InchiKey: IKZQWNAAUFTQOB-UHFFFAOYSA-N
Formula: C24H26F4O4
SMILES: O=C(CCCCCCCCC(=O)OCc1cc(F)ccc1F)OCc1cc(F)ccc1F
Mol. weight [g/mol]: 454.45

Physical Properties

Property code	Value	Unit	Source
gf	-909.58	kJ/mol	Joback Method
hf	-1385.55	kJ/mol	Joback Method
hfus	62.34	kJ/mol	Joback Method
hvap	91.26	kJ/mol	Joback Method
log10ws	-8.12		Crippen Method
logp	6.150		Crippen Method
mcvol	323.460	ml/mol	McGowan Method
pc	1105.21	kPa	Joback Method
rinpol	2903.00		NIST Webbook
rinpol	2903.00		NIST Webbook
tb	971.46	K	Joback Method
tc	1189.37	K	Joback Method
tf	609.84	K	Joback Method
vc	1.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1041.21	J/mol×K	971.46	Joback Method
cpg	1054.31	J/mol×K	1007.78	Joback Method
cpg	1066.05	J/mol×K	1044.10	Joback Method
cpg	1076.45	J/mol×K	1080.41	Joback Method
cpg	1085.56	J/mol×K	1116.73	Joback Method
cpg	1093.40	J/mol×K	1153.05	Joback Method
cpg	1100.02	J/mol×K	1189.37	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380769&Units=SI

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