Sebacic acid, 4-isopropoxyphenyl pentyl ester

Inchi: InChI=1S/C24H38O5/c1-4-5-12-19-27-23(25)13-10-8-6-7-9-11-14-24(26)29-22-17-15-21
InchiKey: PUQOFVLPNIRCLT-UHFFFAOYSA-N
Formula: C24H38O5
SMILES: CCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(OC(C)C)cc1
Mol. weight [g/mol]: 406.56

Physical Properties

Property code	Value	Unit	Source
gf	-321.30	kJ/mol	Joback Method
hf	-940.73	kJ/mol	Joback Method
hfus	54.81	kJ/mol	Joback Method
hvap	92.29	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	6.233		Crippen Method
mcvol	346.010	ml/mol	McGowan Method
pc	1025.31	kPa	Joback Method
rinpol	2911.00		NIST Webbook
tb	954.74	K	Joback Method
tc	1168.99	K	Joback Method
tf	550.73	K	Joback Method
vc	1.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1149.58	J/mol×K	954.74	Joback Method
cpg	1216.09	J/mol×K	1133.28	Joback Method
cpg	1205.77	J/mol×K	1097.57	Joback Method
cpg	1193.99	J/mol×K	1061.87	Joback Method
cpg	1180.71	J/mol×K	1026.16	Joback Method
cpg	1165.91	J/mol×K	990.45	Joback Method
cpg	1224.96	J/mol×K	1168.99	Joback Method
dvisc	0.0000208	Pa×s	954.74	Joback Method
dvisc	0.0000273	Pa×s	887.40	Joback Method

dvisc	0.0000376	Pa×s	820.07	Joback Method
dvisc	0.0000548	Pa×s	752.73	Joback Method
dvisc	0.0000859	Pa×s	685.40	Joback Method
dvisc	0.0001486	Pa×s	618.07	Joback Method
dvisc	0.0002940	Pa×s	550.73	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=U354405&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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