Sebacic acid, 4-isopropoxyphenyl nonyl ester

Inchi: InChI=1S/C28H46O5/c1-4-5-6-7-10-13-16-23-31-27(29)17-14-11-8-9-12-15-18-28(30)33
InchiKey: YRYPVEJXJZOVSO-UHFFFAOYSA-N
Formula: C28H46O5
SMILES: CCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(OC(C)C)cc1
Mol. weight [g/mol]: 462.66

Physical Properties

Property code	Value	Unit	Source
gf	-287.62	kJ/mol	Joback Method
hf	-1023.29	kJ/mol	Joback Method
hfus	65.17	kJ/mol	Joback Method
hvap	101.19	kJ/mol	Joback Method
log10ws	-8.83		Crippen Method
logp	7.794		Crippen Method
mcvol	402.370	ml/mol	McGowan Method
pc	813.07	kPa	Joback Method
rinpol	3327.00		NIST Webbook
rinpol	3327.00		NIST Webbook
tb	1046.26	K	Joback Method
tc	1287.87	K	Joback Method
tf	595.81	K	Joback Method
vc	1.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1398.63	J/mol×K	1046.26	Joback Method
cpg	1415.70	J/mol×K	1086.53	Joback Method
cpg	1430.69	J/mol×K	1126.80	Joback Method
cpg	1443.65	J/mol×K	1167.06	Joback Method
cpg	1454.64	J/mol×K	1207.33	Joback Method
cpg	1463.72	J/mol×K	1247.60	Joback Method
cpg	1470.93	J/mol×K	1287.87	Joback Method
dvisc	0.0001768	Pa×s	595.81	Joback Method

dvisc	0.0000862	Pa×s	670.88	Joback Method
dvisc	0.0000486	Pa×s	745.96	Joback Method
dvisc	0.0000304	Pa×s	821.03	Joback Method
dvisc	0.0000206	Pa×s	896.11	Joback Method
dvisc	0.0000148	Pa×s	971.18	Joback Method
dvisc	0.0000111	Pa×s	1046.26	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=U354410&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
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