Sebacic acid, di(1-phenylpropyl) ester

Inchi: InChI=1S/C28H38O4/c1-3-25(23-17-11-9-12-18-23)31-27(29)21-15-7-5-6-8-16-22-28(30
InchiKey: HHRKKUNYWVKTPG-UHFFFAOYSA-N
Formula: C28H38O4
SMILES: CCC(OC(=O)CCCCCCCCC(=O)OC(CC)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 438.60

Physical Properties

Property code	Value	Unit	Source
gf	-63.02	kJ/mol	Joback Method
hf	-648.35	kJ/mol	Joback Method
hfus	54.89	kJ/mol	Joback Method
hvap	100.01	kJ/mol	Joback Method
log10ws	-8.39		Crippen Method
logp	7.496		Crippen Method
mcvol	372.740	ml/mol	McGowan Method
pc	1016.83	kPa	Joback Method
rinpol	3182.00		NIST Webbook
tb	1045.10	K	Joback Method
tc	1279.73	K	Joback Method
tf	572.48	K	Joback Method
vc	1.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1262.12	J/mol×K	1045.10	Joback Method
cpg	1276.96	J/mol×K	1084.21	Joback Method
cpg	1290.23	J/mol×K	1123.31	Joback Method
cpg	1302.01	J/mol×K	1162.42	Joback Method
cpg	1312.40	J/mol×K	1201.52	Joback Method
cpg	1321.48	J/mol×K	1240.63	Joback Method
cpg	1329.33	J/mol×K	1279.73	Joback Method
dvisc	0.0002866	Pa×s	572.48	Joback Method
dvisc	0.0001277	Pa×s	651.25	Joback Method

dvisc	0.0000678	Pa×s	730.02	Joback Method
dvisc	0.0000407	Pa×s	808.79	Joback Method
dvisc	0.0000267	Pa×s	887.56	Joback Method
dvisc	0.0000188	Pa×s	966.33	Joback Method
dvisc	0.0000140	Pa×s	1045.10	Joback Method

Sources

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=U354994&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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