Sebacic acid, di(2-isopropylphenyl) ester

Inchi: InChI=1S/C28H38O4/c1-21(2)23-15-11-13-17-25(23)31-27(29)19-9-7-5-6-8-10-20-28(30)
InchiKey: WENIXBHBMWHHJJ-UHFFFAOYSA-N
Formula: C28H38O4
SMILES: CC(C)c1ccccc1OC(=O)CCCCCCCCC(=O)Oc1ccccc1C(C)C
Mol. weight [g/mol]: 438.60

Physical Properties

Property code	Value	Unit	Source
gf	-82.28	kJ/mol	Joback Method
hf	-671.29	kJ/mol	Joback Method
hfus	54.11	kJ/mol	Joback Method
hvap	101.33	kJ/mol	Joback Method
log10ws	-8.63		Crippen Method
logp	7.565		Crippen Method
mcvol	372.740	ml/mol	McGowan Method
pc	997.65	kPa	Joback Method
rinpol	3274.00		NIST Webbook
tb	1055.06	K	Joback Method
tc	1291.84	K	Joback Method
tf	597.52	K	Joback Method
vc	1.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1259.91	J/mol×K	1055.06	Joback Method
cpg	1316.05	J/mol×K	1252.38	Joback Method
cpg	1307.88	J/mol×K	1212.91	Joback Method
cpg	1298.24	J/mol×K	1173.45	Joback Method
cpg	1287.09	J/mol×K	1133.99	Joback Method
cpg	1274.33	J/mol×K	1094.52	Joback Method
cpg	1322.85	J/mol×K	1291.84	Joback Method
dvisc	0.0000148	Pa×s	1055.06	Joback Method
dvisc	0.0000194	Pa×s	978.80	Joback Method

dvisc	0.0000268	Pa×s	902.55	Joback Method
dvisc	0.0000392	Pa×s	826.29	Joback Method
dvisc	0.0000620	Pa×s	750.03	Joback Method
dvisc	0.0001088	Pa×s	673.78	Joback Method
dvisc	0.0002202	Pa×s	597.52	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=U354833&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