Sebacic acid, 4-(2-phenylpropyl-2)-phenyl propyl ester

Inchi: InChI=1S/C28H38O4/c1-4-22-31-26(29)16-12-7-5-6-8-13-17-27(30)32-25-20-18-24(19-2

InchiKey: QQWRGALUEPQBCN-UHFFFAOYSA-N

Formula: C28H38O4

SMILES: CCCOC(=O)CCCCCCCCC(=O)Oc1ccc(C(C)(C)c2ccccc2)cc1

Mol. weight [g/mol]: 438.60

Physical Properties

Property code	Value	Unit	Source
gf	-64.93	kJ/mol	Joback Method
hf	-658.01	kJ/mol	Joback Method
hfus	54.13	kJ/mol	Joback Method
hvap	100.15	kJ/mol	Joback Method
log10ws	-7.86		Crippen Method
logp	6.992		Crippen Method
mcvol	372.740	ml/mol	McGowan Method
pc	1009.09	kPa	Joback Method
rinpol	3444.00		NIST Webbook
rinpol	3444.00		NIST Webbook
tb	1047.73	K	Joback Method
tc	1283.24	K	Joback Method
tf	617.42	K	Joback Method
vc	1.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1260.72	J/mol×K	1047.73	Joback Method
cpg	1275.84	J/mol×K	1086.98	Joback Method
cpg	1289.56	J/mol×K	1126.23	Joback Method
cpg	1301.99	J/mol×K	1165.48	Joback Method
cpg	1313.24	J/mol×K	1204.73	Joback Method
cpg	1323.40	J/mol×K	1243.98	Joback Method
cpg	1332.59	J/mol×K	1283.24	Joback Method
dvisc	0.0001784	Pa×s	617.42	Joback Method

dvisc	0.0000918	Pa×s	689.14	Joback Method
dvisc	0.0000536	Pa×s	760.86	Joback Method
dvisc	0.0000343	Pa×s	832.58	Joback Method
dvisc	0.0000236	Pa×s	904.29	Joback Method
dvisc	0.0000171	Pa×s	976.01	Joback Method
dvisc	0.0000130	Pa×s	1047.73	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=U354543&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