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

Inchi: InChI=1S/C29H40O4/c1-4-5-23-32-27(30)17-13-8-6-7-9-14-18-28(31)33-26-21-19-25(20

InchiKey: NXOQVJQKJBUNNZ-UHFFFAOYSA-N

Formula: C29H40O4

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

Mol. weight [g/mol]: 452.63

Physical Properties

Property code	Value	Unit	Source
gf	-56.51	kJ/mol	Joback Method
hf	-678.65	kJ/mol	Joback Method
hfus	56.72	kJ/mol	Joback Method
hvap	102.38	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	7.382		Crippen Method
mcvol	386.830	ml/mol	McGowan Method
pc	950.25	kPa	Joback Method
rinpol	3560.00		NIST Webbook
tb	1070.61	K	Joback Method
tc	1310.73	K	Joback Method
tf	628.69	K	Joback Method
vc	1.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1322.76	J/mol×K	1070.61	Joback Method
cpg	1338.07	J/mol×K	1110.63	Joback Method
cpg	1351.95	J/mol×K	1150.65	Joback Method
cpg	1364.51	J/mol×K	1190.67	Joback Method
cpg	1375.87	J/mol×K	1230.69	Joback Method
cpg	1386.14	J/mol×K	1270.71	Joback Method
cpg	1395.45	J/mol×K	1310.73	Joback Method
dvisc	0.0001563	Pa×s	628.69	Joback Method
dvisc	0.0000797	Pa×s	702.34	Joback Method

dvisc	0.0000462	Pa×s	776.00	Joback Method
dvisc	0.0000295	Pa×s	849.65	Joback Method
dvisc	0.0000202	Pa×s	923.30	Joback Method
dvisc	0.0000146	Pa×s	996.96	Joback Method
dvisc	0.0000111	Pa×s	1070.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354545&Units=SI
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

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