Sebacic acid, isobutyl 1-phenylpropyl ester

Inchi: InChI=1S/C23H36O4/c1-4-21(20-14-10-9-11-15-20)27-23(25)17-13-8-6-5-7-12-16-22(24
InchiKey: GMGDYQDGDOQPSQ-UHFFFAOYSA-N
Formula: C23H36O4
SMILES: CCC(OC(=O)CCCCCCCCC(=O)OCC(C)C)c1ccccc1
Mol. weight [g/mol]: 376.53

Physical Properties

Property code	Value	Unit	Source
gf	-217.53	kJ/mol	Joback Method
hf	-781.68	kJ/mol	Joback Method
hfus	47.89	kJ/mol	Joback Method
hvap	86.60	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	6.001		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1120.80	kPa	Joback Method
rinpol	2625.00		NIST Webbook
tb	904.02	K	Joback Method
tc	1110.67	K	Joback Method
tf	489.71	K	Joback Method
vc	1.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1059.53	J/mol×K	904.02	Joback Method
cpg	1131.47	J/mol×K	1076.23	Joback Method
cpg	1119.57	J/mol×K	1041.78	Joback Method
cpg	1106.46	J/mol×K	1007.34	Joback Method
cpg	1092.11	J/mol×K	972.90	Joback Method
cpg	1076.48	J/mol×K	938.46	Joback Method
cpg	1142.21	J/mol×K	1110.67	Joback Method
dvisc	0.0000293	Pa×s	904.02	Joback Method
dvisc	0.0000396	Pa×s	834.97	Joback Method

dvisc	0.0000567	Pa×s	765.92	Joback Method
dvisc	0.0000872	Pa×s	696.87	Joback Method
dvisc	0.0001473	Pa×s	627.81	Joback Method
dvisc	0.0002833	Pa×s	558.76	Joback Method
dvisc	0.0006550	Pa×s	489.71	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=U354986&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