Sebacic acid, octyl 1-phenylpropyl ester

Inchi: InChI=1S/C27H44O4/c1-3-5-6-7-12-18-23-30-26(28)21-16-10-8-9-11-17-22-27(29)31-25
InchiKey: WQJHPOMKNNGSAP-UHFFFAOYSA-N
Formula: C27H44O4
SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)OC(CC)c1ccccc1
Mol. weight [g/mol]: 432.64

Physical Properties

Property code	Value	Unit	Source
gf	-181.41	kJ/mol	Joback Method
hf	-858.96	kJ/mol	Joback Method
hfus	61.78	kJ/mol	Joback Method
hvap	95.90	kJ/mol	Joback Method
log10ws	-8.41		Crippen Method
logp	7.705		Crippen Method
mcvol	382.410	ml/mol	McGowan Method
pc	875.84	kPa	Joback Method
rinpol	3066.00		NIST Webbook
tb	995.98	K	Joback Method
tc	1220.65	K	Joback Method
tf	549.79	K	Joback Method
vc	1.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1307.33	J/mol×K	995.98	Joback Method
cpg	1325.24	J/mol×K	1033.43	Joback Method
cpg	1341.54	J/mol×K	1070.87	Joback Method
cpg	1356.28	J/mol×K	1108.32	Joback Method
cpg	1369.53	J/mol×K	1145.76	Joback Method
cpg	1381.36	J/mol×K	1183.21	Joback Method
cpg	1391.84	J/mol×K	1220.65	Joback Method
dvisc	0.0003426	Pa×s	549.79	Joback Method
dvisc	0.0001550	Pa×s	624.15	Joback Method

dvisc	0.0000830	Pa×s	698.52	Joback Method
dvisc	0.0000501	Pa×s	772.88	Joback Method
dvisc	0.0000331	Pa×s	847.25	Joback Method
dvisc	0.0000233	Pa×s	921.62	Joback Method
dvisc	0.0000174	Pa×s	995.98	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=U354992&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