Sebacic acid, octyl 3-phenylallyl ester

Inchi: InChI=1S/C27H42O4/c1-2-3-4-5-10-16-23-30-26(28)21-14-8-6-7-9-15-22-27(29)31-24-17
InchiKey: WRJZOXWOUJGOHP-LVZFUZTISA-N
Formula: C27H42O4
SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)OCC=Cc1ccccc1
Mol. weight [g/mol]: 430.62

Physical Properties

Property code	Value	Unit	Source
gf	-98.75	kJ/mol	Joback Method
hf	-736.46	kJ/mol	Joback Method
hfus	65.50	kJ/mol	Joback Method
hvap	96.24	kJ/mol	Joback Method
log10ws	-7.97		Crippen Method
logp	7.268		Crippen Method
mcvol	378.110	ml/mol	McGowan Method
pc	899.10	kPa	Joback Method
rinpol	3309.00		NIST Webbook
rinpol	3309.00		NIST Webbook
tb	1000.58	K	Joback Method
tc	1225.91	K	Joback Method
tf	559.71	K	Joback Method
vc	1.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1278.50	J/mol×K	1000.58	Joback Method
cpg	1296.23	J/mol×K	1038.13	Joback Method
cpg	1312.52	J/mol×K	1075.69	Joback Method
cpg	1327.48	J/mol×K	1113.24	Joback Method
cpg	1341.17	J/mol×K	1150.80	Joback Method
cpg	1353.68	J/mol×K	1188.35	Joback Method
cpg	1365.08	J/mol×K	1225.91	Joback Method
dvisc	0.0002848	Pa×s	559.71	Joback Method

dvisc	0.0001351	Pa×s	633.19	Joback Method
dvisc	0.0000748	Pa×s	706.67	Joback Method
dvisc	0.0000463	Pa×s	780.14	Joback Method
dvisc	0.0000311	Pa×s	853.62	Joback Method
dvisc	0.0000223	Pa×s	927.10	Joback Method
dvisc	0.0000168	Pa×s	1000.58	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355894&Units=SI

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