Sebacic acid, pentyl 3-phenylallyl ester

Inchi: InChI=1S/C24H36O4/c1-2-3-13-20-27-23(25)18-11-6-4-5-7-12-19-24(26)28-21-14-17-22
InchiKey: REOLQHOZIHRLRJ-SAPNQHFASA-N
Formula: C24H36O4
SMILES: CCCCCOC(=O)CCCCCCCCC(=O)OCC=Cc1ccccc1
Mol. weight [g/mol]: 388.54

Physical Properties

Property code	Value	Unit	Source
gf	-124.01	kJ/mol	Joback Method
hf	-674.54	kJ/mol	Joback Method
hfus	57.73	kJ/mol	Joback Method
hvap	89.56	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	6.097		Crippen Method
mcvol	335.840	ml/mol	McGowan Method
pc	1077.10	kPa	Joback Method
rinpol	3010.00		NIST Webbook
tb	931.94	K	Joback Method
tc	1142.39	K	Joback Method
tf	525.90	K	Joback Method
vc	1.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1092.12	J/mol×K	931.94	Joback Method
cpg	1108.84	J/mol×K	967.01	Joback Method
cpg	1124.33	J/mol×K	1002.09	Joback Method
cpg	1138.65	J/mol×K	1037.16	Joback Method
cpg	1151.84	J/mol×K	1072.24	Joback Method
cpg	1163.98	J/mol×K	1107.31	Joback Method
cpg	1175.11	J/mol×K	1142.39	Joback Method
dvisc	0.0004125	Pa×s	525.90	Joback Method
dvisc	0.0002010	Pa×s	593.57	Joback Method

dvisc	0.0001135	Pa×s	661.25	Joback Method
dvisc	0.0000712	Pa×s	728.92	Joback Method
dvisc	0.0000484	Pa×s	796.59	Joback Method
dvisc	0.0000349	Pa×s	864.27	Joback Method
dvisc	0.0000264	Pa×s	931.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355890&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