Sebacic acid, 3-phenylallyl propyl ester

Inchi: InChI=1S/C22H32O4/c1-2-18-25-21(23)16-10-5-3-4-6-11-17-22(24)26-19-12-15-20-13-8
InchiKey: KRBXQYHJJKGMSK-NTCAYCPXSA-N
Formula: C22H32O4
SMILES: CCCOC(=O)CCCCCCCCC(=O)OCC=Cc1ccccc1
Mol. weight [g/mol]: 360.49

Physical Properties

Property code	Value	Unit	Source
gf	-140.85	kJ/mol	Joback Method
hf	-633.26	kJ/mol	Joback Method
hfus	52.55	kJ/mol	Joback Method
hvap	85.11	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	5.317		Crippen Method
mcvol	307.660	ml/mol	McGowan Method
pc	1226.84	kPa	Joback Method
rinpol	2791.00		NIST Webbook
tb	886.18	K	Joback Method
tc	1091.44	K	Joback Method
tf	503.36	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.69	J/mol×K	886.18	Joback Method
cpg	986.89	J/mol×K	920.39	Joback Method
cpg	1001.96	J/mol×K	954.60	Joback Method
cpg	1015.92	J/mol×K	988.81	Joback Method
cpg	1028.84	J/mol×K	1023.02	Joback Method
cpg	1040.76	J/mol×K	1057.23	Joback Method
cpg	1051.72	J/mol×K	1091.44	Joback Method
dvisc	0.0005199	Pa×s	503.36	Joback Method
dvisc	0.0002584	Pa×s	567.16	Joback Method

dvisc	0.0001479	Pa×s	630.97	Joback Method
dvisc	0.0000938	Pa×s	694.77	Joback Method
dvisc	0.0000642	Pa×s	758.57	Joback Method
dvisc	0.0000467	Pa×s	822.38	Joback Method
dvisc	0.0000355	Pa×s	886.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355887&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