Sebacic acid, heptyl 3-phenylallyl ester

Inchi: InChI=1S/C26H40O4/c1-2-3-4-9-15-22-29-25(27)20-13-7-5-6-8-14-21-26(28)30-23-16-19
InchiKey: SZZFTEMAEOTPFR-KNTRCKAVSA-N
Formula: C26H40O4
SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)OCC=Cc1ccccc1
Mol. weight [g/mol]: 416.59

Physical Properties

Property code	Value	Unit	Source
gf	-107.17	kJ/mol	Joback Method
hf	-715.82	kJ/mol	Joback Method
hfus	62.91	kJ/mol	Joback Method
hvap	94.02	kJ/mol	Joback Method
log10ws	-7.55		Crippen Method
logp	6.877		Crippen Method
mcvol	364.020	ml/mol	McGowan Method
pc	953.19	kPa	Joback Method
rinpol	3209.00		NIST Webbook
rinpol	3209.00		NIST Webbook
tb	977.70	K	Joback Method
tc	1197.03	K	Joback Method
tf	548.44	K	Joback Method
vc	1.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1215.88	J/mol×K	977.70	Joback Method
cpg	1289.83	J/mol×K	1160.47	Joback Method
cpg	1277.45	J/mol×K	1123.92	Joback Method
cpg	1263.94	J/mol×K	1087.36	Joback Method
cpg	1249.22	J/mol×K	1050.81	Joback Method
cpg	1233.23	J/mol×K	1014.25	Joback Method
cpg	1301.14	J/mol×K	1197.03	Joback Method
dvisc	0.0000195	Pa×s	977.70	Joback Method

dvisc	0.0000259	Pa×s	906.16	Joback Method
dvisc	0.0000361	Pa×s	834.61	Joback Method
dvisc	0.0000536	Pa×s	763.07	Joback Method
dvisc	0.0000861	Pa×s	691.53	Joback Method
dvisc	0.0001546	Pa×s	619.98	Joback Method
dvisc	0.0003232	Pa×s	548.44	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=U355893&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