Sebacic acid, butyl 3-phenylallyl ester

Inchi: InChI=1S/C23H34O4/c1-2-3-19-26-22(24)17-11-6-4-5-7-12-18-23(25)27-20-13-16-21-14
InchiKey: BQPJIXZFEXUBAZ-DTQAZKPQSA-N
Formula: C23H34O4
SMILES: CCCCOC(=O)CCCCCCCCC(=O)OCC=Cc1ccccc1
Mol. weight [g/mol]: 374.51

Physical Properties

Property code	Value	Unit	Source
gf	-132.43	kJ/mol	Joback Method
hf	-653.90	kJ/mol	Joback Method
hfus	55.14	kJ/mol	Joback Method
hvap	87.34	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	5.707		Crippen Method
mcvol	321.750	ml/mol	McGowan Method
pc	1148.32	kPa	Joback Method
rinpol	2902.00		NIST Webbook
tb	909.06	K	Joback Method
tc	1116.49	K	Joback Method
tf	514.63	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.09	J/mol×K	909.06	Joback Method
cpg	1047.54	J/mol×K	943.63	Joback Method
cpg	1062.81	J/mol×K	978.20	Joback Method
cpg	1076.95	J/mol×K	1012.77	Joback Method
cpg	1090.00	J/mol×K	1047.34	Joback Method
cpg	1102.03	J/mol×K	1081.91	Joback Method
cpg	1113.08	J/mol×K	1116.49	Joback Method
dvisc	0.0004639	Pa×s	514.63	Joback Method
dvisc	0.0002282	Pa×s	580.37	Joback Method

dvisc	0.0001297	Pa×s	646.11	Joback Method
dvisc	0.0000819	Pa×s	711.85	Joback Method
dvisc	0.0000558	Pa×s	777.58	Joback Method
dvisc	0.0000404	Pa×s	843.32	Joback Method
dvisc	0.0000307	Pa×s	909.06	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=U355889&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