Sebacic acid, nonyl 3-phenylallyl ester

Inchi: InChI=1S/C28H44O4/c1-2-3-4-5-8-11-17-24-31-27(29)22-15-9-6-7-10-16-23-28(30)32-25
InchiKey: HVYBMHPGNHEPFL-DYTRJAOYSA-N
Formula: C28H44O4
SMILES: CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCC=Cc1ccccc1
Mol. weight [g/mol]: 444.65

Physical Properties

Property code	Value	Unit	Source
gf	-90.33	kJ/mol	Joback Method
hf	-757.10	kJ/mol	Joback Method
hfus	68.09	kJ/mol	Joback Method
hvap	98.47	kJ/mol	Joback Method
log10ws	-8.39		Crippen Method
logp	7.658		Crippen Method
mcvol	392.200	ml/mol	McGowan Method
pc	849.49	kPa	Joback Method
rinpol	3412.00		NIST Webbook
rinpol	3412.00		NIST Webbook
tb	1023.46	K	Joback Method
tc	1255.93	K	Joback Method
tf	570.98	K	Joback Method
vc	1.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1341.57	J/mol×K	1023.46	Joback Method
cpg	1359.71	J/mol×K	1062.20	Joback Method
cpg	1376.35	J/mol×K	1100.95	Joback Method
cpg	1391.56	J/mol×K	1139.69	Joback Method
cpg	1405.46	J/mol×K	1178.44	Joback Method
cpg	1418.11	J/mol×K	1217.18	Joback Method
cpg	1429.64	J/mol×K	1255.93	Joback Method
dvisc	0.0002504	Pa×s	570.98	Joback Method

dvisc	0.0001177	Pa×s	646.39	Joback Method
dvisc	0.0000648	Pa×s	721.81	Joback Method
dvisc	0.0000399	Pa×s	797.22	Joback Method
dvisc	0.0000268	Pa×s	872.63	Joback Method
dvisc	0.0000191	Pa×s	948.05	Joback Method
dvisc	0.0000143	Pa×s	1023.46	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=U355895&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

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