

Sebacic acid, nonyl 3-phenylpropyl ester

Inchi:	InChI=1S/C28H46O4/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:	SDAZUIJBDODFHM-UHFFFAOYSA-N
Formula:	C28H46O4
SMILES:	CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	446.66

Physical Properties

Property code	Value	Unit	Source
gf	-170.55	kJ/mol	Joback Method
hf	-874.32	kJ/mol	Joback Method
hfus	67.89	kJ/mol	Joback Method
hvap	98.51	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	7.577		Crippen Method
mcvol	396.500	ml/mol	McGowan Method
pc	824.31	kPa	Joback Method
rinsol	3401.00		NIST Webbook
tb	1019.30	K	Joback Method
tc	1252.65	K	Joback Method
tf	576.06	K	Joback Method
vc	1.544	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1370.19	J/molxK	1019.30	Joback Method
cpg	1388.60	J/molxK	1058.19	Joback Method
cpg	1405.27	J/molxK	1097.08	Joback Method
cpg	1420.28	J/molxK	1135.98	Joback Method
cpg	1433.72	J/molxK	1174.87	Joback Method
cpg	1445.65	J/molxK	1213.76	Joback Method
cpg	1456.16	J/molxK	1252.65	Joback Method
dvisc	0.0002698	Paxs	576.06	Joback Method
dvisc	0.0001296	Paxs	649.93	Joback Method

dvisc	0.0000723	Paxs	723.81	Joback Method
dvisc	0.0000449	Paxs	797.68	Joback Method
dvisc	0.0000303	Paxs	871.55	Joback Method
dvisc	0.0000217	Paxs	945.43	Joback Method
dvisc	0.0000163	Paxs	1019.30	Joback Method

Sources

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=U354393&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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