

Sebacic acid, 2,3-dimethylphenyl nonyl ester

Inchi:	InChI=1S/C27H44O4/c1-4-5-6-7-10-13-16-22-30-26(28)20-14-11-8-9-12-15-21-27(29)31
InchiKey:	FNIHVJFIEBXMIW-UHFFFAOYSA-N
Formula:	C27H44O4
SMILES:	CCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]:	432.64

Physical Properties

Property code	Value	Unit	Source
gf	-198.23	kJ/mol	Joback Method
hf	-876.62	kJ/mol	Joback Method
hfus	64.52	kJ/mol	Joback Method
hvap	97.61	kJ/mol	Joback Method
log10ws	-8.72		Crippen Method
logp	7.623		Crippen Method
mvol	382.410	ml/mol	McGowan Method
pc	856.47	kPa	Joback Method
rinpol	3252.00		NIST Webbook
tb	1006.38	K	Joback Method
tc	1234.43	K	Joback Method
tf	589.83	K	Joback Method
vc	1.488	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1305.87	J/molxK	1006.38	Joback Method
cpg	1323.61	J/molxK	1044.39	Joback Method
cpg	1339.66	J/molxK	1082.40	Joback Method
cpg	1354.07	J/molxK	1120.40	Joback Method
cpg	1366.88	J/molxK	1158.41	Joback Method
cpg	1378.16	J/molxK	1196.42	Joback Method
cpg	1387.94	J/molxK	1234.43	Joback Method
dvisc	0.0002371	Paxs	589.83	Joback Method
dvisc	0.0001265	Paxs	659.25	Joback Method

dvisc	0.0000760	Paxs	728.68	Joback Method
dvisc	0.0000500	Paxs	798.10	Joback Method
dvisc	0.0000351	Paxs	867.53	Joback Method
dvisc	0.0000260	Paxs	936.95	Joback Method
dvisc	0.0000201	Paxs	1006.38	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=U355212&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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