Sebacic acid, 3,4-dimethylphenyl nonyl ester

Inchi: InChI=1S/C27H44O4/c1-4-5-6-7-10-13-16-21-30-26(28)17-14-11-8-9-12-15-18-27(29)31
InchiKey: VMMAYZARTMGXJQ-UHFFFAOYSA-N
Formula: C27H44O4
SMILES: CCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(C)c(C)c1
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
mcvol	382.410	ml/mol	McGowan Method
pc	856.47	kPa	Joback Method
rinpol	3320.00		NIST Webbook
tb	1006.38	K	Joback Method
tc	1234.43	K	Joback Method
tf	589.83	K	Joback Method
vc	1.488	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0000760	Pa×s	728.68	Joback Method
dvisc	0.0000500	Pa×s	798.10	Joback Method
dvisc	0.0000351	Pa×s	867.53	Joback Method
dvisc	0.0000260	Pa×s	936.95	Joback Method
dvisc	0.0000201	Pa×s	1006.38	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=U354585&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