Sebacic acid, 3-methylphenyl nonyl ester

Inchi: InChI=1S/C26H42O4/c1-3-4-5-6-9-12-15-21-29-25(27)19-13-10-7-8-11-14-20-26(28)30-2
InchiKey: XHYBSDLOOSBPMJ-UHFFFAOYSA-N
Formula: C26H42O4
SMILES: CCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1cccc(C)c1
Mol. weight [g/mol]: 418.61

Physical Properties

Property code	Value	Unit	Source
gf	-197.02	kJ/mol	Joback Method
hf	-844.51	kJ/mol	Joback Method
hfus	62.32	kJ/mol	Joback Method
hvap	94.72	kJ/mol	Joback Method
log10ws	-8.24		Crippen Method
logp	7.315		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	914.94	kPa	Joback Method
rinpol	3174.00		NIST Webbook
tb	978.52	K	Joback Method
tc	1198.52	K	Joback Method
tf	566.04	K	Joback Method
vc	1.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1243.68	J/mol×K	978.52	Joback Method
cpg	1261.26	J/mol×K	1015.19	Joback Method
cpg	1277.29	J/mol×K	1051.85	Joback Method
cpg	1291.83	J/mol×K	1088.52	Joback Method
cpg	1304.93	J/mol×K	1125.19	Joback Method
cpg	1316.64	J/mol×K	1161.85	Joback Method
cpg	1327.00	J/mol×K	1198.52	Joback Method
dvisc	0.0003036	Pa×s	566.04	Joback Method
dvisc	0.0001561	Pa×s	634.79	Joback Method

dvisc	0.0000914	Pa×s	703.53	Joback Method
dvisc	0.0000589	Pa×s	772.28	Joback Method
dvisc	0.0000407	Pa×s	841.03	Joback Method
dvisc	0.0000298	Pa×s	909.77	Joback Method
dvisc	0.0000228	Pa×s	978.52	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=U354931&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