Sebacic acid, 3,4-dimethylphenyl octyl ester

Inchi: InChI=1S/C26H42O4/c1-4-5-6-7-12-15-20-29-25(27)16-13-10-8-9-11-14-17-26(28)30-24
InchiKey: ZLCJZSZDLDTCMZ-UHFFFAOYSA-N
Formula: C26H42O4
SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(C)c(C)c1
Mol. weight [g/mol]: 418.61

Physical Properties

Property code	Value	Unit	Source
gf	-206.65	kJ/mol	Joback Method
hf	-855.98	kJ/mol	Joback Method
hfus	61.93	kJ/mol	Joback Method
hvap	95.38	kJ/mol	Joback Method
log10ws	-8.30		Crippen Method
logp	7.233		Crippen Method
mcvol	368.320	ml/mol	McGowan Method
pc	906.70	kPa	Joback Method
rinpol	3218.00		NIST Webbook
tb	983.50	K	Joback Method
tc	1204.69	K	Joback Method
tf	578.56	K	Joback Method
vc	1.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1243.12	J/mol×K	983.50	Joback Method
cpg	1315.02	J/mol×K	1167.83	Joback Method
cpg	1303.62	J/mol×K	1130.96	Joback Method
cpg	1290.78	J/mol×K	1094.10	Joback Method
cpg	1276.44	J/mol×K	1057.23	Joback Method
cpg	1260.57	J/mol×K	1020.37	Joback Method
cpg	1325.02	J/mol×K	1204.69	Joback Method
dvisc	0.0000233	Pa×s	983.50	Joback Method
dvisc	0.0000302	Pa×s	916.01	Joback Method

dvisc	0.0000406	Pa×s	848.52	Joback Method
dvisc	0.0000576	Pa×s	781.03	Joback Method
dvisc	0.0000872	Pa×s	713.54	Joback Method
dvisc	0.0001440	Pa×s	646.05	Joback Method
dvisc	0.0002672	Pa×s	578.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354584&Units=SI
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

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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