Sebacic acid, 2,3-dimethylphenyl octyl ester

Inchi: InChI=1S/C26H42O4/c1-4-5-6-7-12-15-21-29-25(27)19-13-10-8-9-11-14-20-26(28)30-24
InchiKey: MWCMIKVPEBWRHR-UHFFFAOYSA-N
Formula: C26H42O4
SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1cccc(C)c1C
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	3143.00		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	1260.57	J/mol×K	1020.37	Joback Method
cpg	1276.44	J/mol×K	1057.23	Joback Method
cpg	1290.78	J/mol×K	1094.10	Joback Method
cpg	1303.62	J/mol×K	1130.96	Joback Method
cpg	1315.02	J/mol×K	1167.83	Joback Method
cpg	1325.02	J/mol×K	1204.69	Joback Method
dvisc	0.0002672	Pa×s	578.56	Joback Method
dvisc	0.0001440	Pa×s	646.05	Joback Method

dvisc	0.0000872	Pa×s	713.54	Joback Method
dvisc	0.0000576	Pa×s	781.03	Joback Method
dvisc	0.0000406	Pa×s	848.52	Joback Method
dvisc	0.0000302	Pa×s	916.01	Joback Method
dvisc	0.0000233	Pa×s	983.50	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=U355211&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