Sebacic acid, decyl 2,3-dimethylphenyl ester

Inchi: InChI=1S/C28H46O4/c1-4-5-6-7-8-11-14-17-23-31-27(29)21-15-12-9-10-13-16-22-28(30)
InchiKey: DRMPYLXJIVMQOY-UHFFFAOYSA-N
Formula: C28H46O4
SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]: 446.66

Physical Properties

Property code	Value	Unit	Source
gf	-189.81	kJ/mol	Joback Method
hf	-897.26	kJ/mol	Joback Method
hfus	67.11	kJ/mol	Joback Method
hvap	99.83	kJ/mol	Joback Method
log10ws	-9.13		Crippen Method
logp	8.014		Crippen Method
mcvol	396.500	ml/mol	McGowan Method
pc	810.30	kPa	Joback Method
rinpol	3353.00		NIST Webbook
tb	1029.26	K	Joback Method
tc	1265.35	K	Joback Method
tf	601.10	K	Joback Method
vc	1.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1368.97	J/mol×K	1029.26	Joback Method
cpg	1387.04	J/mol×K	1068.61	Joback Method
cpg	1403.28	J/mol×K	1107.96	Joback Method
cpg	1417.75	J/mol×K	1147.31	Joback Method
cpg	1430.51	J/mol×K	1186.65	Joback Method
cpg	1441.62	J/mol×K	1226.00	Joback Method
cpg	1451.15	J/mol×K	1265.35	Joback Method
dvisc	0.0002098	Pa×s	601.10	Joback Method
dvisc	0.0001109	Pa×s	672.46	Joback Method

dvisc	0.0000662	Pa×s	743.82	Joback Method
dvisc	0.0000433	Pa×s	815.18	Joback Method
dvisc	0.0000303	Pa×s	886.54	Joback Method
dvisc	0.0000223	Pa×s	957.90	Joback Method
dvisc	0.0000172	Pa×s	1029.26	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=U355213&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