Sebacic acid, dodecyl 2-methylbenzyl ester

Inchi: InChI=1S/C30H50O4/c1-3-4-5-6-7-8-9-12-15-20-25-33-29(31)23-16-13-10-11-14-17-24-3
InchiKey: YPGJHQKWIIUGPY-UHFFFAOYSA-N
Formula: C30H50O4
SMILES: CCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCc1ccccc1C
Mol. weight [g/mol]: 474.72

Physical Properties

Property code	Value	Unit	Source
gf	-163.34	kJ/mol	Joback Method
hf	-927.07	kJ/mol	Joback Method
hfus	72.68	kJ/mol	Joback Method
hvap	103.62	kJ/mol	Joback Method
log10ws	-9.76		Crippen Method
logp	8.623		Crippen Method
mcvol	424.680	ml/mol	McGowan Method
pc	734.42	kPa	Joback Method
rinpol	3305.00		NIST Webbook
rinpol	3305.00		NIST Webbook
tb	1070.04	K	Joback Method
tc	1324.57	K	Joback Method
tf	611.12	K	Joback Method
vc	1.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1496.84	J/mol×K	1070.04	Joback Method
cpg	1515.88	J/mol×K	1112.46	Joback Method
cpg	1532.83	J/mol×K	1154.88	Joback Method
cpg	1547.78	J/mol×K	1197.31	Joback Method
cpg	1560.83	J/mol×K	1239.73	Joback Method
cpg	1572.09	J/mol×K	1282.15	Joback Method
cpg	1581.64	J/mol×K	1324.57	Joback Method
dvisc	0.0001828	Pa×s	611.12	Joback Method

dvisc	0.0000907	Pa×s	687.61	Joback Method
dvisc	0.0000517	Pa×s	764.09	Joback Method
dvisc	0.0000327	Pa×s	840.58	Joback Method
dvisc	0.0000223	Pa×s	917.07	Joback Method
dvisc	0.0000161	Pa×s	993.55	Joback Method
dvisc	0.0000122	Pa×s	1070.04	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=U380722&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