Sebacic acid, 3,5-dimethylphenyl propyl ester

Inchi: InChI=1S/C21H32O4/c1-4-13-24-20(22)11-9-7-5-6-8-10-12-21(23)25-19-15-17(2)14-18(3
InchiKey: QZEZSYLNTIFVGK-UHFFFAOYSA-N
Formula: C21H32O4
SMILES: CCCOC(=O)CCCCCCCCC(=O)Oc1cc(C)cc(C)c1
Mol. weight [g/mol]: 348.48

Physical Properties

Property code	Value	Unit	Source
gf	-248.75	kJ/mol	Joback Method
hf	-752.78	kJ/mol	Joback Method
hfus	48.98	kJ/mol	Joback Method
hvap	84.25	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.283		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1238.96	kPa	Joback Method
rinpol	2636.00		NIST Webbook
rinpol	2636.00		NIST Webbook
tb	869.10	K	Joback Method
tc	1071.22	K	Joback Method
tf	522.21	K	Joback Method
vc	1.151	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	936.55	J/mol×K	869.10	Joback Method
cpg	952.81	J/mol×K	902.79	Joback Method
cpg	967.89	J/mol×K	936.47	Joback Method
cpg	981.80	J/mol×K	970.16	Joback Method
cpg	994.57	J/mol×K	1003.85	Joback Method
cpg	1006.22	J/mol×K	1037.54	Joback Method
cpg	1016.76	J/mol×K	1071.22	Joback Method
dvisc	0.0004628	Pa×s	522.21	Joback Method

dvisc	0.0002633	Pa×s	580.02	Joback Method
dvisc	0.0001659	Pa×s	637.84	Joback Method
dvisc	0.0001129	Pa×s	695.65	Joback Method
dvisc	0.0000815	Pa×s	753.47	Joback Method
dvisc	0.0000616	Pa×s	811.28	Joback Method
dvisc	0.0000484	Pa×s	869.10	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=U354589&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