Sebacic acid, 3,4-dimethylphenyl ethyl ester

Inchi: InChI=1S/C20H30O4/c1-4-23-19(21)11-9-7-5-6-8-10-12-20(22)24-18-14-13-16(2)17(3)15
InchiKey: AQQXJFCXCHWLEJ-UHFFFAOYSA-N
Formula: C20H30O4
SMILES: CCOC(=O)CCCCCCCCC(=O)Oc1ccc(C)c(C)c1
Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
gf	-257.17	kJ/mol	Joback Method
hf	-732.14	kJ/mol	Joback Method
hfus	46.39	kJ/mol	Joback Method
hvap	82.03	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	4.893		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1327.14	kPa	Joback Method
rinpol	2599.00		NIST Webbook
tb	846.22	K	Joback Method
tc	1047.10	K	Joback Method
tf	510.94	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.09	J/mol×K	846.22	Joback Method
cpg	946.18	J/mol×K	1013.62	Joback Method
cpg	934.55	J/mol×K	980.14	Joback Method
cpg	921.85	J/mol×K	946.66	Joback Method
cpg	908.05	J/mol×K	913.18	Joback Method
cpg	893.13	J/mol×K	879.70	Joback Method
cpg	956.74	J/mol×K	1047.10	Joback Method
dvisc	0.0000555	Pa×s	846.22	Joback Method
dvisc	0.0000705	Pa×s	790.34	Joback Method

dvisc	0.0000929	Pa×s	734.46	Joback Method
dvisc	0.0001280	Pa×s	678.58	Joback Method
dvisc	0.0001869	Pa×s	622.70	Joback Method
dvisc	0.0002940	Pa×s	566.82	Joback Method
dvisc	0.0005107	Pa×s	510.94	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=U354576&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