Sebacic acid, ethyl 3-methylphenyl ester

Inchi: InChI=1S/C19H28O4/c1-3-22-18(20)13-8-6-4-5-7-9-14-19(21)23-17-12-10-11-16(2)15-17
InchiKey: AVBMCIZMSQBAMB-UHFFFAOYSA-N
Formula: C19H28O4
SMILES: CCOC(=O)CCCCCCCCC(=O)Oc1cccc(C)c1
Mol. weight [g/mol]: 320.42

Physical Properties

Property code	Value	Unit	Source
gf	-255.96	kJ/mol	Joback Method
hf	-700.03	kJ/mol	Joback Method
hfus	44.19	kJ/mol	Joback Method
hvap	79.14	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.584		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1441.35	kPa	Joback Method
rinpol	2445.00		NIST Webbook
tb	818.36	K	Joback Method
tc	1017.87	K	Joback Method
tf	487.15	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	819.06	J/mol×K	818.36	Joback Method
cpg	834.97	J/mol×K	851.61	Joback Method
cpg	849.80	J/mol×K	884.86	Joback Method
cpg	863.56	J/mol×K	918.12	Joback Method
cpg	876.27	J/mol×K	951.37	Joback Method
cpg	887.96	J/mol×K	984.62	Joback Method
cpg	898.65	J/mol×K	1017.87	Joback Method
dvisc	0.0006541	Pa×s	487.15	Joback Method
dvisc	0.0003630	Pa×s	542.35	Joback Method

dvisc	0.0002246	Pa×s	597.55	Joback Method
dvisc	0.0001507	Pa×s	652.75	Joback Method
dvisc	0.0001077	Pa×s	707.96	Joback Method
dvisc	0.0000807	Pa×s	763.16	Joback Method
dvisc	0.0000629	Pa×s	818.36	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=U354922&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

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