Sebacic acid, 4-formylphenyl isobutyl ester

Inchi: InChI=1S/C21H30O5/c1-17(2)16-25-20(23)9-7-5-3-4-6-8-10-21(24)26-19-13-11-18(15-22
InchiKey: KOPYQTXAJOPCLA-UHFFFAOYSA-N
Formula: C21H30O5
SMILES: CC(C)COC(=O)CCCCCCCCC(=O)Oc1ccc(C=O)cc1
Mol. weight [g/mol]: 362.46

Physical Properties

Property code	Value	Unit	Source
gf	-341.08	kJ/mol	Joback Method
hf	-832.17	kJ/mol	Joback Method
hfus	48.14	kJ/mol	Joback Method
hvap	89.92	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.724		Crippen Method
mcvol	299.440	ml/mol	McGowan Method
pc	1328.10	kPa	Joback Method
rinpol	2839.00		NIST Webbook
rinpol	2839.00		NIST Webbook
tb	912.34	K	Joback Method
tc	1121.72	K	Joback Method
tf	536.69	K	Joback Method
vc	1.163	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	953.31	J/mol×K	912.34	Joback Method
cpg	967.87	J/mol×K	947.24	Joback Method
cpg	981.18	J/mol×K	982.13	Joback Method
cpg	993.29	J/mol×K	1017.03	Joback Method
cpg	1004.20	J/mol×K	1051.93	Joback Method
cpg	1013.96	J/mol×K	1086.83	Joback Method
cpg	1022.59	J/mol×K	1121.72	Joback Method
dvisc	0.0005594	Pa×s	536.69	Joback Method

dvisc	0.0002979	Pa×s	599.30	Joback Method
dvisc	0.0001787	Pa×s	661.91	Joback Method
dvisc	0.0001171	Pa×s	724.51	Joback Method
dvisc	0.0000821	Pa×s	787.12	Joback Method
dvisc	0.0000606	Pa×s	849.73	Joback Method
dvisc	0.0000467	Pa×s	912.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354886&Units=SI
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

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