Sebacic acid, 4-formylphenyl hexyl ester

Inchi: InChI=1S/C23H34O5/c1-2-3-4-11-18-27-22(25)12-9-7-5-6-8-10-13-23(26)28-21-16-14-20
InchiKey: KTHPBQGJSBLFMD-UHFFFAOYSA-N
Formula: C23H34O5
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(C=O)cc1
Mol. weight [g/mol]: 390.51

Physical Properties

Property code	Value	Unit	Source
gf	-321.80	kJ/mol	Joback Method
hf	-868.17	kJ/mol	Joback Method
hfus	56.84	kJ/mol	Joback Method
hvap	94.76	kJ/mol	Joback Method
log10ws	-6.75		Crippen Method
logp	5.649		Crippen Method
mcvol	327.620	ml/mol	McGowan Method
pc	1153.78	kPa	Joback Method
rinpol	3112.00		NIST Webbook
tb	958.54	K	Joback Method
tc	1173.80	K	Joback Method
tf	574.23	K	Joback Method
vc	1.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1073.00	J/mol×K	958.54	Joback Method
cpg	1087.97	J/mol×K	994.42	Joback Method
cpg	1101.57	J/mol×K	1030.29	Joback Method
cpg	1113.86	J/mol×K	1066.17	Joback Method
cpg	1124.86	J/mol×K	1102.04	Joback Method
cpg	1134.62	J/mol×K	1137.92	Joback Method
cpg	1143.16	J/mol×K	1173.80	Joback Method
dvisc	0.0004055	Pa×s	574.23	Joback Method
dvisc	0.0002243	Pa×s	638.28	Joback Method

dvisc	0.0001383	Pa×s	702.33	Joback Method
dvisc	0.0000924	Pa×s	766.38	Joback Method
dvisc	0.0000657	Pa×s	830.44	Joback Method
dvisc	0.0000491	Pa×s	894.49	Joback Method
dvisc	0.0000381	Pa×s	958.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354890&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