Sebacic acid, 4-formylphenyl isohexyl ester

Inchi: InChI=1S/C23H34O5/c1-19(2)10-9-17-27-22(25)11-7-5-3-4-6-8-12-23(26)28-21-15-13-20
InchiKey: HARORJGQTQDJOB-UHFFFAOYSA-N
Formula: C23H34O5
SMILES: CC(C)CCCOC(=O)CCCCCCCCC(=O)Oc1ccc(C=O)cc1
Mol. weight [g/mol]: 390.51

Physical Properties

Property code	Value	Unit	Source
gf	-324.24	kJ/mol	Joback Method
hf	-873.45	kJ/mol	Joback Method
hfus	53.32	kJ/mol	Joback Method
hvap	94.37	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	5.505		Crippen Method
mcvol	327.620	ml/mol	McGowan Method
pc	1160.08	kPa	Joback Method
rinpol	3071.00		NIST Webbook
rinpol	3071.00		NIST Webbook
tb	958.10	K	Joback Method
tc	1173.62	K	Joback Method
tf	559.23	K	Joback Method
vc	1.274	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1073.42	J/mol×K	958.10	Joback Method
cpg	1088.36	J/mol×K	994.02	Joback Method
cpg	1101.92	J/mol×K	1029.94	Joback Method
cpg	1114.15	J/mol×K	1065.86	Joback Method
cpg	1125.07	J/mol×K	1101.78	Joback Method
cpg	1134.74	J/mol×K	1137.70	Joback Method
cpg	1143.18	J/mol×K	1173.62	Joback Method
dvisc	0.0004445	Pa×s	559.23	Joback Method

dvisc	0.0002319	Pa×s	625.71	Joback Method
dvisc	0.0001371	Pa×s	692.19	Joback Method
dvisc	0.0000888	Pa×s	758.66	Joback Method
dvisc	0.0000618	Pa×s	825.14	Joback Method
dvisc	0.0000453	Pa×s	891.62	Joback Method
dvisc	0.0000347	Pa×s	958.10	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354889&Units=SI

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