Sebacic acid, 4-formylphenyl nonyl ester

Inchi: InChI=1S/C26H40O5/c1-2-3-4-5-8-11-14-21-30-25(28)15-12-9-6-7-10-13-16-26(29)31-24
InchiKey: LDVQTLSRHXSKOL-UHFFFAOYSA-N
Formula: C26H40O5
SMILES: CCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(C=O)cc1
Mol. weight [g/mol]: 432.59

Physical Properties

Property code	Value	Unit	Source
gf	-296.54	kJ/mol	Joback Method
hf	-930.09	kJ/mol	Joback Method
hfus	64.61	kJ/mol	Joback Method
hvap	101.44	kJ/mol	Joback Method
log10ws	-8.01		Crippen Method
logp	6.819		Crippen Method
mcvol	369.890	ml/mol	McGowan Method
pc	957.32	kPa	Joback Method
rinpol	3424.00		NIST Webbook
tb	1027.18	K	Joback Method
tc	1260.40	K	Joback Method
tf	608.04	K	Joback Method
vc	1.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1256.96	J/mol×K	1027.18	Joback Method
cpg	1272.70	J/mol×K	1066.05	Joback Method
cpg	1286.78	J/mol×K	1104.92	Joback Method
cpg	1299.26	J/mol×K	1143.79	Joback Method
cpg	1310.21	J/mol×K	1182.66	Joback Method
cpg	1319.68	J/mol×K	1221.53	Joback Method
cpg	1327.74	J/mol×K	1260.40	Joback Method
dvisc	0.0002834	Pa×s	608.04	Joback Method
dvisc	0.0001522	Pa×s	677.90	Joback Method

dvisc	0.0000918	Pa×s	747.75	Joback Method
dvisc	0.0000603	Pa×s	817.61	Joback Method
dvisc	0.0000424	Pa×s	887.47	Joback Method
dvisc	0.0000313	Pa×s	957.32	Joback Method
dvisc	0.0000241	Pa×s	1027.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354893&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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