Sebacic acid, decyl 4-formylphenyl ester

Inchi: InChI=1S/C27H42O5/c1-2-3-4-5-6-9-12-15-22-31-26(29)16-13-10-7-8-11-14-17-27(30)32
InchiKey: VROJYOBKNXAXPK-UHFFFAOYSA-N
Formula: C27H42O5
SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(C=O)cc1
Mol. weight [g/mol]: 446.62

Physical Properties

Property code	Value	Unit	Source
gf	-288.12	kJ/mol	Joback Method
hf	-950.73	kJ/mol	Joback Method
hfus	67.20	kJ/mol	Joback Method
hvap	103.67	kJ/mol	Joback Method
log10ws	-8.42		Crippen Method
logp	7.209		Crippen Method
mcvol	383.980	ml/mol	McGowan Method
pc	902.89	kPa	Joback Method
rinpol	3534.00		NIST Webbook
rinpol	3534.00		NIST Webbook
tb	1050.06	K	Joback Method
tc	1291.61	K	Joback Method
tf	619.31	K	Joback Method
vc	1.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1319.07	J/mol×K	1050.06	Joback Method
cpg	1382.09	J/mol×K	1251.35	Joback Method
cpg	1372.78	J/mol×K	1211.09	Joback Method
cpg	1361.89	J/mol×K	1170.83	Joback Method
cpg	1349.35	J/mol×K	1130.58	Joback Method
cpg	1335.11	J/mol×K	1090.32	Joback Method
cpg	1389.90	J/mol×K	1291.61	Joback Method
dvisc	0.0000207	Pa×s	1050.06	Joback Method

dvisc	0.0000269	Pa×s	978.27	Joback Method
dvisc	0.0000365	Pa×s	906.48	Joback Method
dvisc	0.0000521	Pa×s	834.68	Joback Method
dvisc	0.0000797	Pa×s	762.89	Joback Method
dvisc	0.0001331	Pa×s	691.10	Joback Method
dvisc	0.0002502	Pa×s	619.31	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=U354894&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

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