Sebacic acid, decyl 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C28H46O6/c1-4-5-6-7-8-11-14-17-23-33-26(29)21-15-12-9-10-13-16-22-27(30)
InchiKey: IMUVPYUUDAINGN-UHFFFAOYSA-N
Formula: C28H46O6
SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1c(OC)cccc1OC
Mol. weight [g/mol]: 478.66

Physical Properties

Property code	Value	Unit	Source
gf	-399.81	kJ/mol	Joback Method
hf	-1161.70	kJ/mol	Joback Method
hfus	69.49	kJ/mol	Joback Method
hvap	104.65	kJ/mol	Joback Method
log10ws	-8.42		Crippen Method
logp	7.414		Crippen Method
mcvol	408.240	ml/mol	McGowan Method
pc	794.84	kPa	Joback Method
rinpol	3576.00		NIST Webbook
tb	1074.10	K	Joback Method
tc	1328.71	K	Joback Method
tf	645.56	K	Joback Method
vc	1.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1424.96	J/mol×K	1074.10	Joback Method
cpg	1478.06	J/mol×K	1286.27	Joback Method
cpg	1472.46	J/mol×K	1243.84	Joback Method
cpg	1464.38	J/mol×K	1201.40	Joback Method
cpg	1453.79	J/mol×K	1158.97	Joback Method
cpg	1440.66	J/mol×K	1116.53	Joback Method
cpg	1481.20	J/mol×K	1328.71	Joback Method
dvisc	0.0000092	Pa×s	1074.10	Joback Method
dvisc	0.0000119	Pa×s	1002.68	Joback Method

dvisc	0.0000160	Pa×s	931.25	Joback Method
dvisc	0.0000226	Pa×s	859.83	Joback Method
dvisc	0.0000339	Pa×s	788.41	Joback Method
dvisc	0.0000553	Pa×s	716.98	Joback Method
dvisc	0.0001002	Pa×s	645.56	Joback Method

Sources

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=U354758&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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