

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:	CCCCCCCCCOC(=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
rinpola	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0000160	Paxs	931.25	Joback Method
dvisc	0.0000226	Paxs	859.83	Joback Method
dvisc	0.0000339	Paxs	788.41	Joback Method
dvisc	0.0000553	Paxs	716.98	Joback Method
dvisc	0.0001002	Paxs	645.56	Joback Method

Sources

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
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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