

Sebacic acid, 2,6-dimethoxyphenyl propyl ester

Inchi:	InChI=1S/C21H32O6/c1-4-16-26-19(22)14-9-7-5-6-8-10-15-20(23)27-21-17(24-2)12-11-3
InchiKey:	YFZWJXFAATWQNS-UHFFFAOYSA-N
Formula:	C21H32O6
SMILES:	CCCOC(=O)CCCCCCCCC(=O)Oc1c(OC)cccc1OC
Mol. weight [g/mol]:	380.48

Physical Properties

Property code	Value	Unit	Source
gf	-458.75	kJ/mol	Joback Method
hf	-1017.22	kJ/mol	Joback Method
hfus	51.36	kJ/mol	Joback Method
hvap	89.07	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.683		Crippen Method
mcvol	309.610	ml/mol	McGowan Method
pc	1209.83	kPa	Joback Method
rinqol	2831.00		NIST Webbook
tb	913.94	K	Joback Method
tc	1121.17	K	Joback Method
tf	566.67	K	Joback Method
vc	1.188	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	995.18	J/molxK	913.94	Joback Method
cpg	1010.29	J/molxK	948.48	Joback Method
cpg	1023.97	J/molxK	983.02	Joback Method
cpg	1036.21	J/molxK	1017.56	Joback Method
cpg	1047.02	J/molxK	1052.09	Joback Method
cpg	1056.37	J/molxK	1086.63	Joback Method
cpg	1064.28	J/molxK	1121.17	Joback Method
dvisc	0.0002304	Paxs	566.67	Joback Method
dvisc	0.0001366	Paxs	624.55	Joback Method

dvisc	0.0000884	Paxs	682.43	Joback Method
dvisc	0.0000613	Paxs	740.31	Joback Method
dvisc	0.0000448	Paxs	798.18	Joback Method
dvisc	0.0000342	Paxs	856.06	Joback Method
dvisc	0.0000270	Paxs	913.94	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=U354749&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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