

Sebacic acid, 2,6-dimethoxyphenyl hexyl ester

Inchi:	InChI=1S/C24H38O6/c1-4-5-6-13-19-29-22(25)17-11-9-7-8-10-12-18-23(26)30-24-20(27
InchiKey:	AXBIZMPXDYPLPE-UHFFFAOYSA-N
Formula:	C24H38O6
SMILES:	CCCCCOC(=O)CCCCCCCC(=O)Oc1c(OC)cccc1OC
Mol. weight [g/mol]:	422.55

Physical Properties

Property code	Value	Unit	Source
gf	-433.49	kJ/mol	Joback Method
hf	-1079.14	kJ/mol	Joback Method
hfus	59.13	kJ/mol	Joback Method
hvap	95.75	kJ/mol	Joback Method
log10ws	-6.75		Crippen Method
logp	5.853		Crippen Method
mvol	351.880	ml/mol	McGowan Method
pc	999.54	kPa	Joback Method
rinpol	3143.00		NIST Webbook
rinpol	3143.00		NIST Webbook
tb	982.58	K	Joback Method
tc	1203.34	K	Joback Method
tf	600.48	K	Joback Method
vc	1.355	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1177.42	J/molxK	982.58	Joback Method
cpg	1192.84	J/molxK	1019.37	Joback Method
cpg	1206.49	J/molxK	1056.17	Joback Method
cpg	1218.36	J/molxK	1092.96	Joback Method
cpg	1228.45	J/molxK	1129.75	Joback Method
cpg	1236.77	J/molxK	1166.55	Joback Method
cpg	1243.32	J/molxK	1203.34	Joback Method
dvisc	0.0001641	Paxs	600.48	Joback Method

dvisc	0.0000941	Paxs	664.16	Joback Method
dvisc	0.0000595	Paxs	727.85	Joback Method
dvisc	0.0000405	Paxs	791.53	Joback Method
dvisc	0.0000292	Paxs	855.21	Joback Method
dvisc	0.0000220	Paxs	918.90	Joback Method
dvisc	0.0000172	Paxs	982.58	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=U354754&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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

Latest version available from:

<https://www.chemeo.com/cid/51-308-3/Sebacic-acid-2-6-dimethoxyphenyl-hexyl-ester.pdf>

Generated by Cheméo on 2024-04-26 14:24:05.566560664 +0000 UTC m=+16430694.487137979.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.