

Sebacic acid, 2,6-dimethoxyphenyl ethyl ester

Inchi:	InChI=1S/C20H30O6/c1-4-25-18(21)14-9-7-5-6-8-10-15-19(22)26-20-16(23-2)12-11-13-
InchiKey:	MFPLOSIVIOHSFB-UHFFFAOYSA-N
Formula:	C20H30O6
SMILES:	CCOC(=O)CCCCCCCC(=O)Oc1c(OC)cccc1OC
Mol. weight [g/mol]:	366.45

Physical Properties

Property code	Value	Unit	Source
gf	-467.17	kJ/mol	Joback Method
hf	-996.58	kJ/mol	Joback Method
hfus	48.77	kJ/mol	Joback Method
hvap	86.85	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.293		Crippen Method
mcvol	295.520	ml/mol	McGowan Method
pc	1294.86	kPa	Joback Method
rinpola	2732.00		NIST Webbook
tb	891.06	K	Joback Method
tc	1095.64	K	Joback Method
tf	555.40	K	Joback Method
vc	1.131	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	935.42	J/molxK	891.06	Joback Method
cpg	996.85	J/molxK	1061.54	Joback Method
cpg	987.28	J/molxK	1027.45	Joback Method
cpg	976.34	J/molxK	993.35	Joback Method
cpg	964.04	J/molxK	959.25	Joback Method
cpg	950.40	J/molxK	925.16	Joback Method
cpg	1005.05	J/molxK	1095.64	Joback Method
dvisc	0.0000312	Paxs	891.06	Joback Method
dvisc	0.0000394	Paxs	835.12	Joback Method

dvisc	0.0000515	Paxs	779.17	Joback Method
dvisc	0.0000700	Paxs	723.23	Joback Method
dvisc	0.0001004	Paxs	667.29	Joback Method
dvisc	0.0001537	Paxs	611.34	Joback Method
dvisc	0.0002563	Paxs	555.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354748&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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