

Sebacic acid, 2,6-dimethoxyphenyl isohexyl ester

Inchi:	InChI=1S/C24H38O6/c1-19(2)13-12-18-29-22(25)16-9-7-5-6-8-10-17-23(26)30-24-20(27
InchiKey:	GBCUGJJTZUGPIS-UHFFFAOYSA-N
Formula:	C24H38O6
SMILES:	COc1cccc(OC)c1OC(=O)CCCCCCCC(=O)OCCCC(C)C
Mol. weight [g/mol]:	422.55

Physical Properties

Property code	Value	Unit	Source
gf	-435.93	kJ/mol	Joback Method
hf	-1084.42	kJ/mol	Joback Method
hfus	55.61	kJ/mol	Joback Method
hvap	95.36	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	5.709		Crippen Method
mvol	351.880	ml/mol	McGowan Method
pc	1004.62	kPa	Joback Method
rinpol	3107.00		NIST Webbook
tb	982.14	K	Joback Method
tc	1202.53	K	Joback Method
tf	585.48	K	Joback Method
vc	1.349	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1177.79	J/molxK	982.14	Joback Method
cpg	1236.69	J/molxK	1165.80	Joback Method
cpg	1228.48	J/molxK	1129.07	Joback Method
cpg	1218.48	J/molxK	1092.34	Joback Method
cpg	1206.71	J/molxK	1055.60	Joback Method
cpg	1193.14	J/molxK	1018.87	Joback Method
cpg	1243.14	J/molxK	1202.53	Joback Method
dvisc	0.0000157	Paxs	982.14	Joback Method
dvisc	0.0000203	Paxs	916.03	Joback Method

dvisc	0.0000274	Paxs	849.92	Joback Method
dvisc	0.0000388	Paxs	783.81	Joback Method
dvisc	0.0000587	Paxs	717.70	Joback Method
dvisc	0.0000965	Paxs	651.59	Joback Method
dvisc	0.0001776	Paxs	585.48	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354753&Units=SI

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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