

Sebacic acid, 2,6-dimethoxyphenyl isobutyl ester

Inchi:	InChI=1S/C22H34O6/c1-17(2)16-27-20(23)14-9-7-5-6-8-10-15-21(24)28-22-18(25-3)12-
InchiKey:	TUWPXKBCVGBSMR-UHFFFAOYSA-N
Formula:	C22H34O6
SMILES:	COc1cccc(OC)c1OC(=O)CCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]:	394.50

Physical Properties

Property code	Value	Unit	Source
gf	-452.77	kJ/mol	Joback Method
hf	-1043.14	kJ/mol	Joback Method
hfus	50.43	kJ/mol	Joback Method
hvap	90.91	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.929		Crippen Method
mcvol	323.700	ml/mol	McGowan Method
pc	1139.03	kPa	Joback Method
rinqol	2878.00		NIST Webbook
tb	936.38	K	Joback Method
tc	1147.57	K	Joback Method
tf	562.94	K	Joback Method
vc	1.238	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1055.92	J/molxK	936.38	Joback Method
cpg	1116.49	J/molxK	1112.37	Joback Method
cpg	1107.49	J/molxK	1077.17	Joback Method
cpg	1096.93	J/molxK	1041.97	Joback Method
cpg	1084.81	J/molxK	1006.78	Joback Method
cpg	1071.14	J/molxK	971.58	Joback Method
cpg	1123.93	J/molxK	1147.57	Joback Method
dvisc	0.0000212	Paxs	936.38	Joback Method
dvisc	0.0000273	Paxs	874.14	Joback Method

dvisc	0.0000366	Paxs	811.90	Joback Method
dvisc	0.0000515	Paxs	749.66	Joback Method
dvisc	0.0000770	Paxs	687.42	Joback Method
dvisc	0.0001247	Paxs	625.18	Joback Method
dvisc	0.0002248	Paxs	562.94	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=U354750&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

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