

Sebacic acid, isobutyl 4-isopropoxyphenyl ester

Inchi:	InChI=1S/C23H36O5/c1-18(2)17-26-22(24)11-9-7-5-6-8-10-12-23(25)28-21-15-13-20(14)
InchiKey:	WWZURHKTHGBGRQ-UHFFFAOYSA-N
Formula:	C23H36O5
SMILES:	CC(C)COC(=O)CCCCCCCCC(=O)Oc1ccc(OC(C)C)cc1
Mol. weight [g/mol]:	392.53

Physical Properties

Property code	Value	Unit	Source
gf	-332.16	kJ/mol	Joback Method
hf	-925.37	kJ/mol	Joback Method
hfus	48.69	kJ/mol	Joback Method
hvap	89.68	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	5.699		Crippen Method
mcvol	331.920	ml/mol	McGowan Method
pc	1097.17	kPa	Joback Method
rinpola	2757.00		NIST Webbook
tb	931.42	K	Joback Method
tc	1142.07	K	Joback Method
tf	524.46	K	Joback Method
vc	1.270	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1088.71	J/molxK	931.42	Joback Method
cpg	1104.90	J/molxK	966.53	Joback Method
cpg	1119.62	J/molxK	1001.64	Joback Method
cpg	1132.89	J/molxK	1036.75	Joback Method
cpg	1144.73	J/molxK	1071.85	Joback Method
cpg	1155.16	J/molxK	1106.96	Joback Method
cpg	1164.20	J/molxK	1142.07	Joback Method
dvisc	0.0003723	Paxs	524.46	Joback Method
dvisc	0.0001775	Paxs	592.29	Joback Method

dvisc	0.0000985	Paxs	660.11	Joback Method
dvisc	0.0000610	Paxs	727.94	Joback Method
dvisc	0.0000410	Paxs	795.77	Joback Method
dvisc	0.0000294	Paxs	863.59	Joback Method
dvisc	0.0000221	Paxs	931.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354403&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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