

Sebacic acid, butyl 4-isopropoxyphenyl ester

Inchi:	InChI=1S/C23H36O5/c1-4-5-18-26-22(24)12-10-8-6-7-9-11-13-23(25)28-21-16-14-20(15)
InchiKey:	UJXZHKLDABZQDW-UHFFFAOYSA-N
Formula:	C23H36O5
SMILES:	CCCCOC(=O)CCCCCCCC(=O)Oc1ccc(OC(C)C)cc1
Mol. weight [g/mol]:	392.53

Physical Properties

Property code	Value	Unit	Source
gf	-329.72	kJ/mol	Joback Method
hf	-920.09	kJ/mol	Joback Method
hfus	52.22	kJ/mol	Joback Method
hvap	90.06	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	5.843		Crippen Method
mcvol	331.920	ml/mol	McGowan Method
pc	1091.38	kPa	Joback Method
rinpol	2806.00		NIST Webbook
tb	931.86	K	Joback Method
tc	1141.96	K	Joback Method
tf	539.46	K	Joback Method
vc	1.276	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1088.27	J/molxK	931.86	Joback Method
cpg	1104.46	J/molxK	966.88	Joback Method
cpg	1119.19	J/molxK	1001.89	Joback Method
cpg	1132.49	J/molxK	1036.91	Joback Method
cpg	1144.38	J/molxK	1071.93	Joback Method
cpg	1154.88	J/molxK	1106.95	Joback Method
cpg	1164.02	J/molxK	1141.96	Joback Method
dvisc	0.0003316	Paxs	539.46	Joback Method
dvisc	0.0001693	Paxs	604.86	Joback Method

dvisc	0.0000985	Paxs	670.26	Joback Method
dvisc	0.0000631	Paxs	735.66	Joback Method
dvisc	0.0000435	Paxs	801.06	Joback Method
dvisc	0.0000317	Paxs	866.46	Joback Method
dvisc	0.0000242	Paxs	931.86	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=U354404&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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