

Succinic acid, 2-isopropoxyphenyl 4-isopropylphenyl ester

Inchi:	InChI=1S/C22H26O5/c1-15(2)17-9-11-18(12-10-17)26-21(23)13-14-22(24)27-20-8-6-5-7
InchiKey:	UHV BOLBUHNWEFP-UHFFFAOYSA-N
Formula:	C22H26O5
SMILES:	CC(C)Oc1ccccc1OC(=O)CCC(=O)Oc1ccc(C(C)C)cc1
Mol. weight [g/mol]:	370.44

Physical Properties

Property code	Value	Unit	Source
gf	-237.80	kJ/mol	Joback Method
hf	-679.67	kJ/mol	Joback Method
hfus	39.76	kJ/mol	Joback Method
hvap	90.39	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	4.888		Crippen Method
mcvol	294.070	ml/mol	McGowan Method
pc	1471.36	kPa	Joback Method
rinqol	2792.00		NIST Webbook
tb	940.20	K	Joback Method
tc	1167.22	K	Joback Method
tf	552.13	K	Joback Method
vc	1.105	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	925.14	J/molxK	940.20	Joback Method
cpg	938.67	J/molxK	978.04	Joback Method
cpg	950.66	J/molxK	1015.87	Joback Method
cpg	961.13	J/molxK	1053.71	Joback Method
cpg	970.11	J/molxK	1091.54	Joback Method
cpg	977.62	J/molxK	1129.38	Joback Method
cpg	983.68	J/molxK	1167.22	Joback Method
dvisc	0.0003123	Paxs	552.13	Joback Method
dvisc	0.0001675	Paxs	616.81	Joback Method

dvisc	0.0001011	Paxs	681.49	Joback Method
dvisc	0.0000666	Paxs	746.16	Joback Method
dvisc	0.0000469	Paxs	810.84	Joback Method
dvisc	0.0000348	Paxs	875.52	Joback Method
dvisc	0.0000269	Paxs	940.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357974&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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