

Succinic acid, 2-methylpent-3-yl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C19H28O5/c1-6-15(13(2)3)23-18(20)11-12-19(21)24-17-10-8-7-9-16(17)22-14
InchiKey: ICGJPOZCIHBDIA-UHFFFAOYSA-N
Formula: C19H28O5
SMILES: CCC(OC(=O)CCC(=O)Oc1ccccc1OC(C)C)C(C)C
Mol. weight [g/mol]: 336.42

Physical Properties

Property code	Value	Unit	Source
gf	-368.28	kJ/mol	Joback Method
hf	-848.09	kJ/mol	Joback Method
hfus	34.81	kJ/mol	Joback Method
hvap	80.38	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.137		Crippen Method
mcvol	275.560	ml/mol	McGowan Method
pc	1449.04	kPa	Joback Method
rinpol	2199.00		NIST Webbook
rinpol	2199.00		NIST Webbook
tb	839.46	K	Joback Method
tc	1045.65	K	Joback Method
tf	464.38	K	Joback Method
vc	1.040	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.74	J/molxK	839.46	Joback Method
cpg	865.60	J/molxK	873.83	Joback Method
cpg	880.21	J/molxK	908.19	Joback Method
cpg	893.57	J/molxK	942.56	Joback Method
cpg	905.69	J/molxK	976.92	Joback Method
cpg	916.58	J/molxK	1011.29	Joback Method
cpg	926.26	J/molxK	1045.65	Joback Method
dvisc	0.0006887	Paxs	464.38	Joback Method

dvisc	0.0003157	Paxs	526.89	Joback Method
dvisc	0.0001707	Paxs	589.41	Joback Method
dvisc	0.0001039	Paxs	651.92	Joback Method
dvisc	0.0000689	Paxs	714.43	Joback Method
dvisc	0.0000489	Paxs	776.95	Joback Method
dvisc	0.0000365	Paxs	839.46	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=U389788&Units=SI

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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