

Succinic acid, phenethyl 4-isopropylphenyl ester

Inchi:	InChI=1S/C21H24O4/c1-16(2)18-8-10-19(11-9-18)25-21(23)13-12-20(22)24-15-14-17-6-
InchiKey:	JHFKFNUBAGCTAN-UHFFFAOYSA-N
Formula:	C21H24O4
SMILES:	CC(C)c1ccc(OC(=O)CCC(=O)OCCc2ccccc2)cc1
Mol. weight [g/mol]:	340.41

Physical Properties

Property code	Value	Unit	Source
gf	-129.15	kJ/mol	Joback Method
hf	-510.06	kJ/mol	Joback Method
hfus	39.89	kJ/mol	Joback Method
hvap	85.48	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.281		Crippen Method
mcvol	274.110	ml/mol	McGowan Method
pc	1616.77	kPa	Joback Method
rinpol	2752.00		NIST Webbook
rinpol	2752.00		NIST Webbook
tb	890.36	K	Joback Method
tc	1115.31	K	Joback Method
tf	521.11	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.84	J/mol×K	890.36	Joback Method
cpg	898.87	J/mol×K	1077.81	Joback Method
cpg	889.58	J/mol×K	1040.32	Joback Method
cpg	879.07	J/mol×K	1002.83	Joback Method
cpg	867.30	J/mol×K	965.34	Joback Method
cpg	854.24	J/mol×K	927.85	Joback Method
cpg	907.00	J/mol×K	1115.31	Joback Method
dvisc	0.0000447	Pa×s	890.36	Joback Method

dvisc	0.0000577	Pa×s	828.82	Joback Method
dvisc	0.0000778	Pa×s	767.28	Joback Method
dvisc	0.0001104	Pa×s	705.73	Joback Method
dvisc	0.0001674	Pa×s	644.19	Joback Method
dvisc	0.0002773	Pa×s	582.65	Joback Method
dvisc	0.0005174	Pa×s	521.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358006&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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