Succinic acid, 2-isopropoxyphenyl 2-methoxyethyl ester

Inchi: InChI=1S/C16H22O6/c1-12(2)21-13-6-4-5-7-14(13)22-16(18)9-8-15(17)20-11-10-19-3/h4

InchiKey: AXZBTRPJMWEMNX-UHFFFAOYSA-N

Formula: C16H22O6

SMILES: COCCOC(=O)CCC(=O)Oc1ccccc1OC(C)C

Mol. weight [g/mol]: 310.34

Physical Properties

Property code	Value	Unit	Source
gf	-493.66	kJ/mol	Joback Method
hf	-907.83	kJ/mol	Joback Method
hfus	35.27	kJ/mol	Joback Method
hvap	76.89	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.349		Crippen Method
mcvol	239.160	ml/mol	McGowan Method
pc	1777.34	kPa	Joback Method
rinpol	2182.00		NIST Webbook
rinpol	2182.00		NIST Webbook
tb	794.12	K	Joback Method
tc	997.41	K	Joback Method
tf	482.80	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.70	J/mol×K	794.12	Joback Method
cpg	719.22	J/mol×K	828.00	Joback Method
cpg	732.65	J/mol×K	861.88	Joback Method
cpg	744.97	J/mol×K	895.76	Joback Method
cpg	756.18	J/mol×K	929.64	Joback Method
cpg	766.24	J/mol×K	963.53	Joback Method
cpg	775.16	J/mol×K	997.41	Joback Method
dvisc	0.0004895	Pa×s	482.80	Joback Method

dvisc	0.0002778	Pa×s	534.69	Joback Method
dvisc	0.0001743	Pa×s	586.57	Joback Method
dvisc	0.0001180	Pa×s	638.46	Joback Method
dvisc	0.0000847	Pa×s	690.35	Joback Method
dvisc	0.0000637	Pa×s	742.23	Joback Method
dvisc	0.0000497	Pa×s	794.12	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357966&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