

Succinic acid, 2-isopropoxyphenyl 2-chloroethyl ester

Inchi:	InChI=1S/C15H19ClO5/c1-11(2)20-12-5-3-4-6-13(12)21-15(18)8-7-14(17)19-10-9-16/h3-
InchiKey:	POYYKUSQGBZQIL-UHFFFAOYSA-N
Formula:	C15H19ClO5
SMILES:	CC(C)Oc1ccccc1OC(=O)CCC(=O)OCCCl
Mol. weight [g/mol]:	314.76

Physical Properties

Property code	Value	Unit	Source
gf	-409.01	kJ/mol	Joback Method
hf	-770.71	kJ/mol	Joback Method
hfus	35.69	kJ/mol	Joback Method
hvap	76.64	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	2.941		Crippen Method
mvol	231.440	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
rinpol	2207.00		NIST Webbook
tb	786.25	K	Joback Method
tc	995.37	K	Joback Method
tf	479.22	K	Joback Method
vc	0.876	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.42	J/molxK	786.25	Joback Method
cpg	704.61	J/molxK	960.51	Joback Method
cpg	695.24	J/molxK	925.66	Joback Method
cpg	684.84	J/molxK	890.81	Joback Method
cpg	673.40	J/molxK	855.96	Joback Method
cpg	660.93	J/molxK	821.10	Joback Method
cpg	712.94	J/molxK	995.37	Joback Method
dvisc	0.0000660	Paxs	786.25	Joback Method
dvisc	0.0000843	Paxs	735.08	Joback Method

dvisc	0.0001118	Paxs	683.91	Joback Method
dvisc	0.0001552	Paxs	632.74	Joback Method
dvisc	0.0002282	Paxs	581.56	Joback Method
dvisc	0.0003615	Paxs	530.39	Joback Method
dvisc	0.0006317	Paxs	479.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357967&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

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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