

Succinic acid, 2-isopropoxyphenyl 2-ethoxyethyl ester

Inchi:	InChI=1S/C17H24O6/c1-4-20-11-12-21-16(18)9-10-17(19)23-15-8-6-5-7-14(15)22-13(2)3
InchiKey:	BQJVLDLDERYLTHU-UHFFFAOYSA-N
Formula:	C17H24O6
SMILES:	CCOCCOC(=O)CCC(=O)Oc1ccccc1OC(C)C
Mol. weight [g/mol]:	324.37

Physical Properties

Property code	Value	Unit	Source
gf	-485.24	kJ/mol	Joback Method
hf	-928.47	kJ/mol	Joback Method
hfus	37.86	kJ/mol	Joback Method
hvap	79.12	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.739		Crippen Method
mvol	253.250	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
rinpol	2245.00		NIST Webbook
tb	817.00	K	Joback Method
tc	1019.65	K	Joback Method
tf	494.07	K	Joback Method
vc	0.958	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.51	J/molxK	817.00	Joback Method
cpg	776.24	J/molxK	850.77	Joback Method
cpg	789.82	J/molxK	884.55	Joback Method
cpg	802.23	J/molxK	918.32	Joback Method
cpg	813.47	J/molxK	952.10	Joback Method
cpg	823.53	J/molxK	985.87	Joback Method
cpg	832.40	J/molxK	1019.65	Joback Method
dvisc	0.0004441	Paxs	494.07	Joback Method
dvisc	0.0002489	Paxs	547.89	Joback Method

dvisc	0.0001547	Paxs	601.71	Joback Method
dvisc	0.0001040	Paxs	655.53	Joback Method
dvisc	0.0000742	Paxs	709.36	Joback Method
dvisc	0.0000556	Paxs	763.18	Joback Method
dvisc	0.0000432	Paxs	817.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357969&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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