Succinic acid, 4-iodobenzyl propyl ester

Inchi: InChI=1S/C14H17IO4/c1-2-9-18-13(16)7-8-14(17)19-10-11-3-5-12(15)6-4-11/h3-6H,2,7-1
InchiKey: ZSCFTGYLTBMSIZ-UHFFFAOYSA-N
Formula: C14H17IO4
SMILES: CCCOC(=O)CCC(=O)OCc1ccc(I)cc1
Mol. weight [g/mol]: 376.19

Physical Properties

Property code	Value	Unit	Source
gf	-239.94	kJ/mol	Joback Method
hf	-519.96	kJ/mol	Joback Method
hfus	35.65	kJ/mol	Joback Method
hvap	77.38	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.068		Crippen Method
mcvol	225.060	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	2263.00		NIST Webbook
rinpol	2263.00		NIST Webbook
tb	797.10	K	Joback Method
tc	1024.09	K	Joback Method
tf	488.86	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	588.17	J/mol×K	797.10	Joback Method
cpg	600.78	J/mol×K	834.93	Joback Method
cpg	612.37	J/mol×K	872.76	Joback Method
cpg	622.98	J/mol×K	910.59	Joback Method
cpg	632.62	J/mol×K	948.43	Joback Method
cpg	641.32	J/mol×K	986.26	Joback Method
cpg	649.09	J/mol×K	1024.09	Joback Method
dvisc	0.0007951	Pa×s	488.86	Joback Method

dvisc	0.0004700	Pa×s	540.23	Joback Method
dvisc	0.0003044	Pa×s	591.61	Joback Method
dvisc	0.0002113	Pa×s	642.98	Joback Method
dvisc	0.0001548	Pa×s	694.35	Joback Method
dvisc	0.0001184	Pa×s	745.73	Joback Method
dvisc	0.0000937	Pa×s	797.10	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=U380889&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