Succinic acid, di(2-iodobenzyl) ester

Inchi: InChI=1S/C18H16I2O4/c19-15-7-3-1-5-13(15)11-23-17(21)9-10-18(22)24-12-14-6-2-4-8-
InchiKey: ADNHWKMNJLAVIV-UHFFFAOYSA-N
Formula: C18H16I2O4
SMILES: O=C(CCC(=O)OCc1ccccc1I)OCc1ccccc1I
Mol. weight [g/mol]: 550.13

Physical Properties

Property code	Value	Unit	Source
gf	-45.36	kJ/mol	Joback Method
hf	-300.59	kJ/mol	Joback Method
hfus	44.07	kJ/mol	Joback Method
hvap	98.60	kJ/mol	Joback Method
log10ws	-6.57		Crippen Method
logp	4.463		Crippen Method
mcvol	283.480	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
rinpol	3216.00		NIST Webbook
rinpol	3216.00		NIST Webbook
tb	1013.42	K	Joback Method
tc	1281.32	K	Joback Method
tf	630.94	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.21	J/mol×K	1013.42	Joback Method
cpg	776.27	J/mol×K	1236.67	Joback Method
cpg	771.24	J/mol×K	1192.02	Joback Method
cpg	765.30	J/mol×K	1147.37	Joback Method
cpg	758.38	J/mol×K	1102.72	Joback Method
cpg	750.37	J/mol×K	1058.07	Joback Method
cpg	780.46	J/mol×K	1281.32	Joback Method
dvisc	0.0000370	Pa×s	1013.42	Joback Method

dvisc	0.0000464	Pa×s	949.67	Joback Method
dvisc	0.0000601	Pa×s	885.93	Joback Method
dvisc	0.0000811	Pa×s	822.18	Joback Method
dvisc	0.0001150	Pa×s	758.43	Joback Method
dvisc	0.0001739	Pa×s	694.69	Joback Method
dvisc	0.0002858	Pa×s	630.94	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U381114&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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