Succinic acid, heptyl 3-iodobenzyl ester

Inchi: InChI=1S/C18H25IO4/c1-2-3-4-5-6-12-22-17(20)10-11-18(21)23-14-15-8-7-9-16(19)13-1
InchiKey: FNWPKUFIVZNUEQ-UHFFFAOYSA-N
Formula: C18H25IO4
SMILES: CCCCCCCOC(=O)CCC(=O)OCc1cccc(I)c1
Mol. weight [g/mol]: 432.29

Physical Properties

Property code	Value	Unit	Source
gf	-206.26	kJ/mol	Joback Method
hf	-602.52	kJ/mol	Joback Method
hfus	46.01	kJ/mol	Joback Method
hvap	86.28	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.628		Crippen Method
mcvol	281.420	ml/mol	McGowan Method
pc	1525.88	kPa	Joback Method
rinpol	2651.00		NIST Webbook
rinpol	2651.00		NIST Webbook
tb	888.62	K	Joback Method
tc	1107.61	K	Joback Method
tf	533.94	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.55	J/mol×K	888.62	Joback Method
cpg	826.16	J/mol×K	925.12	Joback Method
cpg	838.65	J/mol×K	961.62	Joback Method
cpg	850.05	J/mol×K	998.12	Joback Method
cpg	860.40	J/mol×K	1034.61	Joback Method
cpg	869.73	J/mol×K	1071.11	Joback Method
cpg	878.08	J/mol×K	1107.61	Joback Method
dvisc	0.0005232	Pa×s	533.94	Joback Method

dvisc	0.0002945	Pa×s	593.05	Joback Method
dvisc	0.0001839	Pa×s	652.17	Joback Method
dvisc	0.0001242	Pa×s	711.28	Joback Method
dvisc	0.0000891	Pa×s	770.39	Joback Method
dvisc	0.0000670	Pa×s	829.51	Joback Method
dvisc	0.0000524	Pa×s	888.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381387&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
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