Succinic acid, 2-iodobenzyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C18H25IO4/c1-4-7-16(13(2)3)23-18(21)11-10-17(20)22-12-14-8-5-6-9-15(14)1

InchiKey: KXZUMGQECVOLMG-UHFFFAOYSA-N

Formula: C18H25IO4

SMILES: CCCC(OC(=O)CCC(=O)OCc1ccccc1I)C(C)C

Mol. weight [g/mol]: 432.29

Physical Properties

Property code	Value	Unit	Source
gf	-211.14	kJ/mol	Joback Method
hf	-613.08	kJ/mol	Joback Method
hfus	38.96	kJ/mol	Joback Method
hvap	85.51	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	4.483		Crippen Method
mcvol	281.420	ml/mol	McGowan Method
pc	1545.13	kPa	Joback Method
rinpol	2498.00		NIST Webbook
rinpol	2498.00		NIST Webbook
tb	887.74	K	Joback Method
tc	1111.68	K	Joback Method
tf	503.94	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.61	J/mol×K	887.74	Joback Method
cpg	871.24	J/mol×K	1074.36	Joback Method
cpg	861.97	J/mol×K	1037.04	Joback Method
cpg	851.60	J/mol×K	999.71	Joback Method
cpg	840.11	J/mol×K	962.39	Joback Method
cpg	827.46	J/mol×K	925.06	Joback Method
cpg	879.47	J/mol×K	1111.68	Joback Method
dvisc	0.0000438	Pa×s	887.74	Joback Method

dvisc	0.0000577	Pa×s	823.77	Joback Method
dvisc	0.0000796	Pa×s	759.81	Joback Method
dvisc	0.0001166	Pa×s	695.84	Joback Method
dvisc	0.0001845	Pa×s	631.87	Joback Method
dvisc	0.0003239	Pa×s	567.91	Joback Method
dvisc	0.0006556	Pa×s	503.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381104&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