Succinic acid, 3-iodobenzyl isobutyl ester

Inchi: InChI=1S/C15H19IO4/c1-11(2)9-19-14(17)6-7-15(18)20-10-12-4-3-5-13(16)8-12/h3-5,8,1
InchiKey: FOVZNGCBELPMJV-UHFFFAOYSA-N
Formula: C15H19IO4
SMILES: CC(C)COC(=O)CCC(=O)OCc1cccc(I)c1
Mol. weight [g/mol]: 390.21

Physical Properties

Property code	Value	Unit	Source
gf	-233.96	kJ/mol	Joback Method
hf	-545.88	kJ/mol	Joback Method
hfus	34.71	kJ/mol	Joback Method
hvap	79.22	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	3.314		Crippen Method
mcvol	239.150	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	2300.00		NIST Webbook
rinpol	2300.00		NIST Webbook
tb	819.54	K	Joback Method
tc	1046.98	K	Joback Method
tf	485.13	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.48	J/mol×K	819.54	Joback Method
cpg	656.58	J/mol×K	857.45	Joback Method
cpg	668.60	J/mol×K	895.35	Joback Method
cpg	679.56	J/mol×K	933.26	Joback Method
cpg	689.49	J/mol×K	971.17	Joback Method
cpg	698.42	J/mol×K	1009.07	Joback Method
cpg	706.37	J/mol×K	1046.98	Joback Method
dvisc	0.0008096	Pa×s	485.13	Joback Method

dvisc	0.0004434	Pa×s	540.87	Joback Method
dvisc	0.0002717	Pa×s	596.60	Joback Method
dvisc	0.0001811	Pa×s	652.34	Joback Method
dvisc	0.0001286	Pa×s	708.07	Joback Method
dvisc	0.0000960	Pa×s	763.80	Joback Method
dvisc	0.0000746	Pa×s	819.54	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=U381382&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