Succinic acid, ethyl 3-iodobenzyl ester

Inchi: InChI=1S/C13H15IO4/c1-2-17-12(15)6-7-13(16)18-9-10-4-3-5-11(14)8-10/h3-5,8H,2,6-7,
InchiKey: SGOAARVYTKPQFG-UHFFFAOYSA-N
Formula: C13H15IO4
SMILES: CCOC(=O)CCC(=O)OCc1cccc(I)c1
Mol. weight [g/mol]: 362.16

Physical Properties

Property code	Value	Unit	Source
gf	-248.36	kJ/mol	Joback Method
hf	-499.32	kJ/mol	Joback Method
hfus	33.06	kJ/mol	Joback Method
hvap	75.16	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	2.678		Crippen Method
mcvol	210.970	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinpol	2145.00		NIST Webbook
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tb	774.22	K	Joback Method
tc	1004.72	K	Joback Method
tf	477.59	K	Joback Method
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.49	J/mol×K	774.22	Joback Method
cpg	586.01	J/mol×K	966.31	Joback Method
cpg	577.59	J/mol×K	927.89	Joback Method
cpg	568.25	J/mol×K	889.47	Joback Method
cpg	557.97	J/mol×K	851.05	Joback Method
cpg	546.72	J/mol×K	812.64	Joback Method
cpg	593.53	J/mol×K	1004.72	Joback Method
dvisc	0.0001078	Pa×s	774.22	Joback Method

dvisc	0.0001356	Pa×s	724.78	Joback Method
dvisc	0.0001765	Pa×s	675.34	Joback Method
dvisc	0.0002395	Pa×s	625.90	Joback Method
dvisc	0.0003424	Pa×s	576.47	Joback Method
dvisc	0.0005234	Pa×s	527.03	Joback Method
dvisc	0.0008737	Pa×s	477.59	Joback Method

Sources

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=U381381&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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