

Succinic acid, di(3-iodobenzyl) ester

Inchi: InChI=1S/C18H16I2O4/c19-15-5-1-3-13(9-15)11-23-17(21)7-8-18(22)24-12-14-4-2-6-16(20-18)
InchiKey: AZELSKKJMGELLZ-UHFFFAOYSA-N
Formula: C18H16I2O4
SMILES: O=C(CCC(=O)OCc1cccc(I)c1)OCc1cccc(I)c1
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
mvol	283.480	ml/mol	McGowan Method
pc	1947.51	kPa	Joback Method
rinpol	3143.00		NIST Webbook
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tb	1013.42	K	Joback Method
tc	1281.32	K	Joback Method
tf	630.94	K	Joback Method
vc	1.052	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.21	J/molxK	1013.42	Joback Method
cpg	750.37	J/molxK	1058.07	Joback Method
cpg	758.38	J/molxK	1102.72	Joback Method
cpg	765.30	J/molxK	1147.37	Joback Method
cpg	771.24	J/molxK	1192.02	Joback Method
cpg	776.27	J/molxK	1236.67	Joback Method
cpg	780.46	J/molxK	1281.32	Joback Method
dvisc	0.0002858	Paxs	630.94	Joback Method

dvisc	0.0001739	Paxs	694.69	Joback Method
dvisc	0.0001150	Paxs	758.43	Joback Method
dvisc	0.0000811	Paxs	822.18	Joback Method
dvisc	0.0000601	Paxs	885.93	Joback Method
dvisc	0.0000464	Paxs	949.67	Joback Method
dvisc	0.0000370	Paxs	1013.42	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U381389&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

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