

Succinic acid, dodecyl 2-iodobenzyl ester

Inchi:	InChI=1S/C23H35IO4/c1-2-3-4-5-6-7-8-9-10-13-18-27-22(25)16-17-23(26)28-19-20-14-1
InchiKey:	NHVUPBHDFEOPX-UHFFFAOYSA-N
Formula:	C23H35IO4
SMILES:	CCCCCCCCCCCCOC(=O)CCC(=O)OCc1ccccc1I
Mol. weight [g/mol]:	502.43

Physical Properties

Property code	Value	Unit	Source
gf	-164.16	kJ/mol	Joback Method
hf	-705.72	kJ/mol	Joback Method
hfus	58.96	kJ/mol	Joback Method
hvap	97.41	kJ/mol	Joback Method
log10ws	-7.92		Crippen Method
logp	6.579		Crippen Method
mvol	351.870	ml/mol	McGowan Method
pc	1082.06	kPa	Joback Method
rinpol	3149.00		NIST Webbook
rinpol	3149.00		NIST Webbook
tb	1003.02	K	Joback Method
tc	1229.00	K	Joback Method
tf	590.29	K	Joback Method
vc	1.351	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1109.79	J/molxK	1003.02	Joback Method
cpg	1169.60	J/molxK	1191.33	Joback Method
cpg	1160.05	J/molxK	1153.67	Joback Method
cpg	1149.36	J/molxK	1116.01	Joback Method
cpg	1137.45	J/molxK	1078.35	Joback Method
cpg	1124.28	J/molxK	1040.68	Joback Method
cpg	1178.04	J/molxK	1229.00	Joback Method
dvisc	0.0000242	Paxs	1003.02	Joback Method

dvisc	0.0000314	Paxs	934.23	Joback Method
dvisc	0.0000425	Paxs	865.44	Joback Method
dvisc	0.0000606	Paxs	796.65	Joback Method
dvisc	0.0000924	Paxs	727.87	Joback Method
dvisc	0.0001536	Paxs	659.08	Joback Method
dvisc	0.0002878	Paxs	590.29	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=U381111&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

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