

Sebacic acid, 3-iodobenzyl pentyl ester

Inchi:	InChI=1S/C22H33IO4/c1-2-3-10-16-26-21(24)14-8-6-4-5-7-9-15-22(25)27-18-19-12-11-1
InchiKey:	AVGGEONFCJRTED-UHFFFAOYSA-N
Formula:	C22H33IO4
SMILES:	CCCCCOC(=O)CCCCCCCC(=O)OCc1cccc(I)c1
Mol. weight [g/mol]:	488.40

Physical Properties

Property code	Value	Unit	Source
gf	-172.58	kJ/mol	Joback Method
hf	-685.08	kJ/mol	Joback Method
hfus	56.37	kJ/mol	Joback Method
hvap	95.19	kJ/mol	Joback Method
log10ws	-7.50		Crippen Method
logp	6.189		Crippen Method
mvol	337.780	ml/mol	McGowan Method
pc	1153.78	kPa	Joback Method
rinpol	3055.00		NIST Webbook
rinpol	3055.00		NIST Webbook
tb	980.14	K	Joback Method
tc	1202.94	K	Joback Method
tf	579.02	K	Joback Method
vc	1.296	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1049.16	J/molxK	980.14	Joback Method
cpg	1063.47	J/molxK	1017.27	Joback Method
cpg	1076.50	J/molxK	1054.41	Joback Method
cpg	1088.32	J/molxK	1091.54	Joback Method
cpg	1098.96	J/molxK	1128.67	Joback Method
cpg	1108.49	J/molxK	1165.80	Joback Method
cpg	1116.95	J/molxK	1202.94	Joback Method
dvisc	0.0003262	Paxs	579.02	Joback Method

dvisc	0.0001759	Paxs	645.87	Joback Method
dvisc	0.0001065	Paxs	712.73	Joback Method
dvisc	0.0000702	Paxs	779.58	Joback Method
dvisc	0.0000495	Paxs	846.43	Joback Method
dvisc	0.0000367	Paxs	913.29	Joback Method
dvisc	0.0000284	Paxs	980.14	Joback Method

Sources

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=U380755&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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