Sebacic acid, 2-iodobenzyl pentyl ester

Inchi: InChI=1S/C22H33IO4/c1-2-3-12-17-26-21(24)15-8-6-4-5-7-9-16-22(25)27-18-19-13-10-1
InchiKey: KKXLVXVRBMMAAZ-UHFFFAOYSA-N
Formula: C22H33IO4
SMILES: CCCCCOC(=O)CCCCCCCCC(=O)OCc1ccccc1I
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
mcvol	337.780	ml/mol	McGowan Method
pc	1153.78	kPa	Joback Method
rinpol	3053.00		NIST Webbook
rinpol	3053.00		NIST Webbook
tb	980.14	K	Joback Method
tc	1202.94	K	Joback Method
tf	579.02	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001759	Pa×s	645.87	Joback Method
dvisc	0.0001065	Pa×s	712.73	Joback Method
dvisc	0.0000702	Pa×s	779.58	Joback Method
dvisc	0.0000495	Pa×s	846.43	Joback Method
dvisc	0.0000367	Pa×s	913.29	Joback Method
dvisc	0.0000284	Pa×s	980.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380672&Units=SI
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

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