Sebacic acid, hexyl 3-iodobenzyl ester

Inchi: InChI=1S/C23H35IO4/c1-2-3-4-11-17-27-22(25)15-9-7-5-6-8-10-16-23(26)28-19-20-13-1
InchiKey: KRQBZADJXLLPTG-UHFFFAOYSA-N
Formula: C23H35IO4
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)OCc1cccc(I)c1
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
mcvol	351.870	ml/mol	McGowan Method
pc	1082.06	kPa	Joback Method
rinpol	3125.00		NIST Webbook
rinpol	3125.00		NIST Webbook
tb	1003.02	K	Joback Method
tc	1229.00	K	Joback Method
tf	590.29	K	Joback Method
vc	1.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1109.79	J/mol×K	1003.02	Joback Method
cpg	1124.28	J/mol×K	1040.68	Joback Method
cpg	1137.45	J/mol×K	1078.35	Joback Method
cpg	1149.36	J/mol×K	1116.01	Joback Method
cpg	1160.05	J/mol×K	1153.67	Joback Method
cpg	1169.60	J/mol×K	1191.33	Joback Method
cpg	1178.04	J/mol×K	1229.00	Joback Method
dvisc	0.0002878	Pa×s	590.29	Joback Method

dvisc	0.0001536	Pa×s	659.08	Joback Method
dvisc	0.0000924	Pa×s	727.87	Joback Method
dvisc	0.0000606	Pa×s	796.65	Joback Method
dvisc	0.0000425	Pa×s	865.44	Joback Method
dvisc	0.0000314	Pa×s	934.23	Joback Method
dvisc	0.0000242	Pa×s	1003.02	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380756&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