Sebacic acid, 2-iodobenzyl octyl ester

Inchi: InChI=1S/C25H39IO4/c1-2-3-4-5-10-15-20-29-24(27)18-11-8-6-7-9-12-19-25(28)30-21-2
InchiKey: LCGGMJZULKFCCG-UHFFFAOYSA-N
Formula: C25H39IO4
SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)OCc1ccccc1I
Mol. weight [g/mol]: 530.48

Physical Properties

Property code	Value	Unit	Source
gf	-147.32	kJ/mol	Joback Method
hf	-747.00	kJ/mol	Joback Method
hfus	64.14	kJ/mol	Joback Method
hvap	101.87	kJ/mol	Joback Method
log10ws	-8.76		Crippen Method
logp	7.359		Crippen Method
mcvol	380.050	ml/mol	McGowan Method
pc	957.32	kPa	Joback Method
rinpol	3250.00		NIST Webbook
rinpol	3250.00		NIST Webbook
tb	1048.78	K	Joback Method
tc	1284.22	K	Joback Method
tf	612.83	K	Joback Method
vc	1.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1232.45	J/mol×K	1048.78	Joback Method
cpg	1293.32	J/mol×K	1244.98	Joback Method
cpg	1283.77	J/mol×K	1205.74	Joback Method
cpg	1272.98	J/mol×K	1166.50	Joback Method
cpg	1260.88	J/mol×K	1127.26	Joback Method
cpg	1247.39	J/mol×K	1088.02	Joback Method
cpg	1301.71	J/mol×K	1284.22	Joback Method
dvisc	0.0000176	Pa×s	1048.78	Joback Method

dvisc	0.0000230	Pa×s	976.12	Joback Method
dvisc	0.0000313	Pa×s	903.46	Joback Method
dvisc	0.0000449	Pa×s	830.80	Joback Method
dvisc	0.0000691	Pa×s	758.15	Joback Method
dvisc	0.0001165	Pa×s	685.49	Joback Method
dvisc	0.0002225	Pa×s	612.83	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=U380675&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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