Sebacic acid, 3-iodo-4-methoxybenzyl propyl ester

Inchi: InChI=1S/C21H31IO5/c1-3-14-26-20(23)10-8-6-4-5-7-9-11-21(24)27-16-17-12-13-19(25-

InchiKey: AAPMRUSDDIAHCW-UHFFFAOYSA-N

Formula: C21H31IO5

SMILES: CCCOC(=O)CCCCCCCCC(=O)OCc1ccc(OC)c(I)c1

Mol. weight [g/mol]: 490.37

Physical Properties

Property code	Value	Unit	Source
gf	-295.63	kJ/mol	Joback Method
hf	-808.13	kJ/mol	Joback Method
hfus	54.58	kJ/mol	Joback Method
hvap	96.04	kJ/mol	Joback Method
log10ws	-6.79		Crippen Method
logp	5.417		Crippen Method
mcvol	329.560	ml/mol	McGowan Method
pc	1205.63	kPa	Joback Method
rinpol	3086.00		NIST Webbook
rinpol	3086.00		NIST Webbook
tb	984.66	K	Joback Method
tc	1208.59	K	Joback Method
tf	602.50	K	Joback Method
vc	1.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1015.25	J/mol×K	984.66	Joback Method
cpg	1028.43	J/mol×K	1021.98	Joback Method
cpg	1040.19	J/mol×K	1059.30	Joback Method
cpg	1050.57	J/mol×K	1096.63	Joback Method
cpg	1059.57	J/mol×K	1133.95	Joback Method
cpg	1067.24	J/mol×K	1171.27	Joback Method
cpg	1073.58	J/mol×K	1208.59	Joback Method
dvisc	0.0002275	Pa×s	602.50	Joback Method

dvisc	0.0001320	Pa×s	666.19	Joback Method
dvisc	0.0000842	Pa×s	729.89	Joback Method
dvisc	0.0000577	Pa×s	793.58	Joback Method
dvisc	0.0000418	Pa×s	857.27	Joback Method
dvisc	0.0000317	Pa×s	920.97	Joback Method
dvisc	0.0000249	Pa×s	984.66	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=U380638&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