Sebacic acid, 4-iodobenzyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C24H37IO4/c1-4-11-22(19(2)3)29-24(27)13-10-8-6-5-7-9-12-23(26)28-18-20-1

InchiKey: ZLMNRJOYKQPJNA-UHFFFAOYSA-N

Formula: C24H37IO4

SMILES: CCCC(OC(=O)CCCCCCCCC(=O)OCc1ccc(I)cc1)C(C)C

Mol. weight [g/mol]: 516.45

Physical Properties

Property code	Value	Unit	Source
gf	-160.62	kJ/mol	Joback Method
hf	-736.92	kJ/mol	Joback Method
hfus	54.50	kJ/mol	Joback Method
hvap	98.86	kJ/mol	Joback Method
log10ws	-8.21		Crippen Method
logp	6.823		Crippen Method
mcvol	365.960	ml/mol	McGowan Method
pc	1027.28	kPa	Joback Method
rinpol	3144.00		NIST Webbook
rinpol	3144.00		NIST Webbook
tb	1025.02	K	Joback Method
tc	1255.64	K	Joback Method
tf	571.56	K	Joback Method
vc	1.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1171.51	J/mol×K	1025.02	Joback Method
cpg	1230.86	J/mol×K	1217.20	Joback Method
cpg	1221.57	J/mol×K	1178.76	Joback Method
cpg	1211.06	J/mol×K	1140.33	Joback Method
cpg	1199.26	J/mol×K	1101.89	Joback Method
cpg	1186.09	J/mol×K	1063.46	Joback Method
cpg	1238.98	J/mol×K	1255.64	Joback Method
dvisc	0.0000171	Pa×s	1025.02	Joback Method

dvisc	0.0000228	Pa×s	949.44	Joback Method
dvisc	0.0000320	Pa×s	873.87	Joback Method
dvisc	0.0000479	Pa×s	798.29	Joback Method
dvisc	0.0000779	Pa×s	722.71	Joback Method
dvisc	0.0001422	Pa×s	647.14	Joback Method
dvisc	0.0003040	Pa×s	571.56	Joback Method

Sources

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=U380627&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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