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

Inchi: InChI=1S/C20H29IO5/c1-3-25-19(22)10-8-6-4-5-7-9-11-20(23)26-15-16-12-13-18(24-2)17(21)14-16/h12-14H,3-11,15H2,1-2H3

InchiKey: LDCAEBUDFNXFCO-UHFFFAOYSA-N

Formula: C20H29IO5

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

Mol. weight [g/mol]: 476.35

Physical Properties

Property code	Value	Unit	Source
gf	-304.05	kJ/mol	Joback Method
hf	-787.49	kJ/mol	Joback Method
hfus	51.99	kJ/mol	Joback Method
hvap	93.81	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	5.027		Crippen Method
mcvol	315.470	ml/mol	McGowan Method
pc	1290.21	kPa	Joback Method
rinpol	3022.00		NIST Webbook
rinpol	3022.00		NIST Webbook
tb	961.78	K	Joback Method
tc	1183.54	K	Joback Method
tf	591.23	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.74	J/mol×K	961.78	Joback Method
cpg	968.83	J/mol×K	998.74	Joback Method
cpg	980.56	J/mol×K	1035.70	Joback Method
cpg	990.97	J/mol×K	1072.66	Joback Method
cpg	1000.07	J/mol×K	1109.62	Joback Method
cpg	1007.88	J/mol×K	1146.58	Joback Method
cpg	1014.41	J/mol×K	1183.54	Joback Method
dvisc	0.0002564	Pa×s	591.23	Joback Method

dvisc	0.0001503	Pa×s	652.99	Joback Method
dvisc	0.0000966	Pa×s	714.75	Joback Method
dvisc	0.0000666	Pa×s	776.50	Joback Method
dvisc	0.0000485	Pa×s	838.26	Joback Method
dvisc	0.0000369	Pa×s	900.02	Joback Method
dvisc	0.0000291	Pa×s	961.78	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=U380637&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