Sebacic acid, ethyl 2-iodobenzyl ester

Inchi: InChI=1S/C19H27IO4/c1-2-23-18(21)13-7-5-3-4-6-8-14-19(22)24-15-16-11-9-10-12-17(1
InchiKey: JUZUIIVAUBWBGS-UHFFFAOYSA-N
Formula: C19H27IO4
SMILES: CCOC(=O)CCCCCCCCC(=O)OCc1ccccc1I
Mol. weight [g/mol]: 446.32

Physical Properties

Property code	Value	Unit	Source
gf	-197.84	kJ/mol	Joback Method
hf	-623.16	kJ/mol	Joback Method
hfus	48.60	kJ/mol	Joback Method
hvap	88.51	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	5.018		Crippen Method
mcvol	295.510	ml/mol	McGowan Method
pc	1417.57	kPa	Joback Method
rinpol	2794.00		NIST Webbook
rinpol	2794.00		NIST Webbook
tb	911.50	K	Joback Method
tc	1130.22	K	Joback Method
tf	545.21	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.71	J/mol×K	911.50	Joback Method
cpg	928.52	J/mol×K	1093.76	Joback Method
cpg	919.11	J/mol×K	1057.31	Joback Method
cpg	908.66	J/mol×K	1020.86	Joback Method
cpg	897.14	J/mol×K	984.41	Joback Method
cpg	884.50	J/mol×K	947.95	Joback Method
cpg	936.92	J/mol×K	1130.22	Joback Method
dvisc	0.0000450	Pa×s	911.50	Joback Method

dvisc	0.0000578	Pa×s	850.45	Joback Method
dvisc	0.0000772	Pa×s	789.40	Joback Method
dvisc	0.0001081	Pa×s	728.36	Joback Method
dvisc	0.0001610	Pa×s	667.31	Joback Method
dvisc	0.0002599	Pa×s	606.26	Joback Method
dvisc	0.0004671	Pa×s	545.21	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=U380668&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