Sebacic acid, 2-iodobenzyl propyl ester

Inchi: InChI=1S/C20H29IO4/c1-2-15-24-19(22)13-7-5-3-4-6-8-14-20(23)25-16-17-11-9-10-12-1
InchiKey: OPBOPTHFGSWNAE-UHFFFAOYSA-N
Formula: C20H29IO4
SMILES: CCCOC(=O)CCCCCCCCC(=O)OCc1ccccc1I
Mol. weight [g/mol]: 460.35

Physical Properties

Property code	Value	Unit	Source
gf	-189.42	kJ/mol	Joback Method
hf	-643.80	kJ/mol	Joback Method
hfus	51.19	kJ/mol	Joback Method
hvap	90.74	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	5.408		Crippen Method
mcvol	309.600	ml/mol	McGowan Method
pc	1320.39	kPa	Joback Method
rinpol	2887.00		NIST Webbook
rinpol	2887.00		NIST Webbook
tb	934.38	K	Joback Method
tc	1153.60	K	Joback Method
tf	556.48	K	Joback Method
vc	1.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	929.57	J/mol×K	934.38	Joback Method
cpg	943.53	J/mol×K	970.92	Joback Method
cpg	956.30	J/mol×K	1007.45	Joback Method
cpg	967.93	J/mol×K	1043.99	Joback Method
cpg	978.46	J/mol×K	1080.53	Joback Method
cpg	987.92	J/mol×K	1117.07	Joback Method
cpg	996.37	J/mol×K	1153.60	Joback Method
dvisc	0.0004156	Pa×s	556.48	Joback Method

dvisc	0.0002288	Pa×s	619.46	Joback Method
dvisc	0.0001406	Pa×s	682.45	Joback Method
dvisc	0.0000938	Pa×s	745.43	Joback Method
dvisc	0.0000667	Pa×s	808.41	Joback Method
dvisc	0.0000498	Pa×s	871.40	Joback Method
dvisc	0.0000387	Pa×s	934.38	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=U380669&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