Sebacic acid, 2-iodobenzyl isobutyl ester

Inchi: InChI=1S/C21H31IO4/c1-17(2)15-25-20(23)13-7-5-3-4-6-8-14-21(24)26-16-18-11-9-10-1
InchiKey: NIGWRFPANADQHQ-UHFFFAOYSA-N
Formula: C21H31IO4
SMILES: CC(C)COC(=O)CCCCCCCCC(=O)OCc1ccccc1I
Mol. weight [g/mol]: 474.37

Physical Properties

Property code	Value	Unit	Source
gf	-183.44	kJ/mol	Joback Method
hf	-669.72	kJ/mol	Joback Method
hfus	50.26	kJ/mol	Joback Method
hvap	92.57	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	5.654		Crippen Method
mcvol	323.690	ml/mol	McGowan Method
pc	1239.83	kPa	Joback Method
rinpol	2935.00		NIST Webbook
rinpol	2935.00		NIST Webbook
tb	956.82	K	Joback Method
tc	1178.71	K	Joback Method
tf	552.75	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.51	J/mol×K	956.82	Joback Method
cpg	1003.67	J/mol×K	993.80	Joback Method
cpg	1016.58	J/mol×K	1030.78	Joback Method
cpg	1028.28	J/mol×K	1067.77	Joback Method
cpg	1038.82	J/mol×K	1104.75	Joback Method
cpg	1048.25	J/mol×K	1141.73	Joback Method
cpg	1056.60	J/mol×K	1178.71	Joback Method
dvisc	0.0004055	Pa×s	552.75	Joback Method

dvisc	0.0002079	Pa×s	620.10	Joback Method
dvisc	0.0001215	Pa×s	687.44	Joback Method
dvisc	0.0000782	Pa×s	754.78	Joback Method
dvisc	0.0000540	Pa×s	822.13	Joback Method
dvisc	0.0000395	Pa×s	889.47	Joback Method
dvisc	0.0000302	Pa×s	956.82	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=U380670&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