Glutaric acid, 3-iodobenzyl pentyl ester

Inchi: InChI=1S/C17H23IO4/c1-2-3-4-11-21-16(19)9-6-10-17(20)22-13-14-7-5-8-15(18)12-14/h
InchiKey: DWIYPMFVGHDUNY-UHFFFAOYSA-N
Formula: C17H23IO4
SMILES: CCCCCOC(=O)CCCC(=O)OCc1cccc(I)c1
Mol. weight [g/mol]: 418.27

Physical Properties

Property code	Value	Unit	Source
gf	-214.68	kJ/mol	Joback Method
hf	-581.88	kJ/mol	Joback Method
hfus	43.42	kJ/mol	Joback Method
hvap	84.06	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.238		Crippen Method
mcvol	267.330	ml/mol	McGowan Method
pc	1647.09	kPa	Joback Method
rinpol	2603.00		NIST Webbook
rinpol	2603.00		NIST Webbook
tb	865.74	K	Joback Method
tc	1085.74	K	Joback Method
tf	522.67	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.15	J/mol×K	865.74	Joback Method
cpg	768.56	J/mol×K	902.41	Joback Method
cpg	780.88	J/mol×K	939.07	Joback Method
cpg	792.14	J/mol×K	975.74	Joback Method
cpg	802.37	J/mol×K	1012.41	Joback Method
cpg	811.59	J/mol×K	1049.07	Joback Method
cpg	819.86	J/mol×K	1085.74	Joback Method
dvisc	0.0005842	Pa×s	522.67	Joback Method

dvisc	0.0003326	Pa×s	579.85	Joback Method
dvisc	0.0002095	Pa×s	637.03	Joback Method
dvisc	0.0001424	Pa×s	694.20	Joback Method
dvisc	0.0001027	Pa×s	751.38	Joback Method
dvisc	0.0000775	Pa×s	808.56	Joback Method
dvisc	0.0000608	Pa×s	865.74	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=U376986&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