Glutaric acid, 3-iodobenzyl isobutyl ester

Inchi: InChI=1S/C16H21IO4/c1-12(2)10-20-15(18)7-4-8-16(19)21-11-13-5-3-6-14(17)9-13/h3,5-
InchiKey: GFSIZMDPUHDVMA-UHFFFAOYSA-N
Formula: C16H21IO4
SMILES: CC(C)COC(=O)CCCC(=O)OCc1cccc(I)c1
Mol. weight [g/mol]: 404.24

Physical Properties

Property code	Value	Unit	Source
gf	-225.54	kJ/mol	Joback Method
hf	-566.52	kJ/mol	Joback Method
hfus	37.30	kJ/mol	Joback Method
hvap	81.44	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	3.704		Crippen Method
mcvol	253.240	ml/mol	McGowan Method
pc	1795.46	kPa	Joback Method
rinpol	2453.00		NIST Webbook
tb	842.42	K	Joback Method
tc	1067.19	K	Joback Method
tf	496.40	K	Joback Method
vc	0.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.15	J/mol×K	842.42	Joback Method
cpg	712.49	J/mol×K	879.88	Joback Method
cpg	724.73	J/mol×K	917.34	Joback Method
cpg	735.89	J/mol×K	954.80	Joback Method
cpg	746.01	J/mol×K	992.27	Joback Method
cpg	755.10	J/mol×K	1029.73	Joback Method
cpg	763.20	J/mol×K	1067.19	Joback Method
dvisc	0.0007277	Pa×s	496.40	Joback Method
dvisc	0.0003938	Pa×s	554.07	Joback Method

dvisc	0.0002392	Pa×s	611.74	Joback Method
dvisc	0.0001584	Pa×s	669.41	Joback Method
dvisc	0.0001119	Pa×s	727.08	Joback Method
dvisc	0.0000833	Pa×s	784.75	Joback Method
dvisc	0.0000645	Pa×s	842.42	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=U376984&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