Glutaric acid, 3-iodobenzyl propyl ester

Inchi: InChI=1S/C15H19IO4/c1-2-9-19-14(17)7-4-8-15(18)20-11-12-5-3-6-13(16)10-12/h3,5-6,1
InchiKey: ZFRIANFBSQGEMH-UHFFFAOYSA-N
Formula: C15H19IO4
SMILES: CCCOC(=O)CCCC(=O)OCc1cccc(I)c1
Mol. weight [g/mol]: 390.21

Physical Properties

Property code	Value	Unit	Source
gf	-231.52	kJ/mol	Joback Method
hf	-540.60	kJ/mol	Joback Method
hfus	38.24	kJ/mol	Joback Method
hvap	79.61	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.458		Crippen Method
mcvol	239.150	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
rinpol	2396.00		NIST Webbook
rinpol	2396.00		NIST Webbook
tb	819.98	K	Joback Method
tc	1044.02	K	Joback Method
tf	500.13	K	Joback Method
vc	0.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	642.89	J/mol×K	819.98	Joback Method
cpg	697.36	J/mol×K	1006.68	Joback Method
cpg	688.44	J/mol×K	969.34	Joback Method
cpg	678.56	J/mol×K	932.00	Joback Method
cpg	667.69	J/mol×K	894.66	Joback Method
cpg	655.81	J/mol×K	857.32	Joback Method
cpg	705.34	J/mol×K	1044.02	Joback Method
dvisc	0.0000813	Pa×s	819.98	Joback Method

dvisc	0.0001031	Pa×s	766.67	Joback Method
dvisc	0.0001354	Pa×s	713.36	Joback Method
dvisc	0.0001858	Pa×s	660.05	Joback Method
dvisc	0.0002696	Pa×s	606.75	Joback Method
dvisc	0.0004203	Pa×s	553.44	Joback Method
dvisc	0.0007203	Pa×s	500.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376983&Units=SI
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

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

Latest version available from:
https://www.chemeo.com/cid/93-618-3/Glutaric-acid-3-iodobenzyl-propyl-ester.pdf
Generated by Cheméo on 2024-10-12 07:28:21.199473012 +0000 UTC m=+3298963.836442260.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.