

Glutaric acid, 2-iodobenzyl isobutyl ester

Inchi:	InChI=1S/C16H21IO4/c1-12(2)10-20-15(18)8-5-9-16(19)21-11-13-6-3-4-7-14(13)17/h3-4
InchiKey:	ZKPWRPXJFVUIST-UHFFFAOYSA-N
Formula:	C16H21IO4
SMILES:	CC(C)COC(=O)CCCC(=O)OCc1ccccc1I
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	2421.00		NIST Webbook
rinpol	2421.00		NIST Webbook
tb	842.42	K	Joback Method
tc	1067.19	K	Joback Method
tf	496.40	K	Joback Method
vc	0.954	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.15	J/molxK	842.42	Joback Method
cpg	712.49	J/molxK	879.88	Joback Method
cpg	724.73	J/molxK	917.34	Joback Method
cpg	735.89	J/molxK	954.80	Joback Method
cpg	746.01	J/molxK	992.27	Joback Method
cpg	755.10	J/molxK	1029.73	Joback Method
cpg	763.20	J/molxK	1067.19	Joback Method
dvisc	0.0007277	Paxs	496.40	Joback Method

dvisc	0.0003938	Paxs	554.07	Joback Method
dvisc	0.0002392	Paxs	611.74	Joback Method
dvisc	0.0001584	Paxs	669.41	Joback Method
dvisc	0.0001119	Paxs	727.08	Joback Method
dvisc	0.0000833	Paxs	784.75	Joback Method
dvisc	0.0000645	Paxs	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=U376877&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

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