

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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	642.89	J/molxK	819.98	Joback Method
cpg	655.81	J/molxK	857.32	Joback Method
cpg	667.69	J/molxK	894.66	Joback Method
cpg	678.56	J/molxK	932.00	Joback Method
cpg	688.44	J/molxK	969.34	Joback Method
cpg	697.36	J/molxK	1006.68	Joback Method
cpg	705.34	J/molxK	1044.02	Joback Method
dvisc	0.0007203	Paxs	500.13	Joback Method

dvisc	0.0004203	Paxs	553.44	Joback Method
dvisc	0.0002696	Paxs	606.75	Joback Method
dvisc	0.0001858	Paxs	660.05	Joback Method
dvisc	0.0001354	Paxs	713.36	Joback Method
dvisc	0.0001031	Paxs	766.67	Joback Method
dvisc	0.0000813	Paxs	819.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376983&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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