

Glutaric acid, ethyl 3-iodobenzyl ester

Inchi:	InChI=1S/C14H17IO4/c1-2-18-13(16)7-4-8-14(17)19-10-11-5-3-6-12(15)9-11/h3,5-6,9H,2
InchiKey:	DG XKRETZBHVFLP-UHFFFAOYSA-N
Formula:	C14H17IO4
SMILES:	CCOC(=O)CCCC(=O)OCc1cccc(I)c1
Mol. weight [g/mol]:	376.19

Physical Properties

Property code	Value	Unit	Source
gf	-239.94	kJ/mol	Joback Method
hf	-519.96	kJ/mol	Joback Method
hfus	35.65	kJ/mol	Joback Method
hvap	77.38	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.068		Crippen Method
mvol	225.060	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	2301.00		NIST Webbook
rinpol	2301.00		NIST Webbook
tb	797.10	K	Joback Method
tc	1024.09	K	Joback Method
tf	488.86	K	Joback Method
vc	0.848	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	588.17	J/mol×K	797.10	Joback Method
cpg	641.32	J/mol×K	986.26	Joback Method
cpg	632.62	J/mol×K	948.43	Joback Method
cpg	622.98	J/mol×K	910.59	Joback Method
cpg	612.37	J/mol×K	872.76	Joback Method
cpg	600.78	J/mol×K	834.93	Joback Method
cpg	649.09	J/mol×K	1024.09	Joback Method
dvisc	0.0000937	Paxs	797.10	Joback Method

dvisc	0.0001184	Paxs	745.73	Joback Method
dvisc	0.0001548	Paxs	694.35	Joback Method
dvisc	0.0002113	Paxs	642.98	Joback Method
dvisc	0.0003044	Paxs	591.61	Joback Method
dvisc	0.0004700	Paxs	540.23	Joback Method
dvisc	0.0007951	Paxs	488.86	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376982&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

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