

Propionic acid, 3-iodo-, pentyl ester

Inchi:	InChI=1S/C8H15IO2/c1-2-3-4-7-11-8(10)5-6-9/h2-7H2,1H3
InchiKey:	TVIQIONYLJULRP-UHFFFAOYSA-N
Formula:	C8H15IO2
SMILES:	CCCCCOC(=O)CI
Mol. weight [g/mol]:	270.11

Physical Properties

Property code	Value	Unit	Source
gf	-159.32	kJ/mol	Joback Method
hf	-376.38	kJ/mol	Joback Method
hfus	23.67	kJ/mol	Joback Method
hvap	51.93	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.545		Crippen Method
mcvol	156.840	ml/mol	McGowan Method
pc	2597.78	kPa	Joback Method
rinpol	1420.00		NIST Webbook
rinpol	1420.00		NIST Webbook
tb	551.87	K	Joback Method
tc	755.24	K	Joback Method
tf	310.14	K	Joback Method
vc	0.596	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.40	J/molxK	551.87	Joback Method
cpg	344.49	J/molxK	585.76	Joback Method
cpg	356.00	J/molxK	619.66	Joback Method
cpg	366.92	J/molxK	653.55	Joback Method
cpg	377.28	J/molxK	687.45	Joback Method
cpg	387.10	J/molxK	721.34	Joback Method
cpg	396.37	J/molxK	755.24	Joback Method
dvisc	0.0033031	Paxs	310.14	Joback Method

dvisc	0.0017028	Paxs	350.43	Joback Method
dvisc	0.0010063	Paxs	390.72	Joback Method
dvisc	0.0006562	Paxs	431.00	Joback Method
dvisc	0.0004603	Paxs	471.29	Joback Method
dvisc	0.0003415	Paxs	511.58	Joback Method
dvisc	0.0002646	Paxs	551.87	Joback Method

Sources

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=U406240&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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