

Alpha-iodo propionic acid

Inchi:	InChI=1S/C3H5IO2/c1-2(4)3(5)6/h2H,1H3,(H,5,6)
InchiKey:	KZLYQYPURWXOEW-UHFFFAOYSA-N
Formula:	C3H5IO2
SMILES:	CC(I)C(=O)O
Mol. weight [g/mol]:	199.98
CAS:	598-80-1

Physical Properties

Property code	Value	Unit	Source
gf	-235.68	kJ/mol	Joback Method
hf	-298.47	kJ/mol	Joback Method
hfus	10.10	kJ/mol	Joback Method
hvap	54.68	kJ/mol	Joback Method
log10ws	-1.24		Crippen Method
logp	0.894		Crippen Method
mcvol	86.390	ml/mol	McGowan Method
pc	5367.04	kPa	Joback Method
tb	506.79	K	Joback Method
tc	717.98	K	Joback Method
tf	277.38	K	Joback Method
vc	0.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	142.87	J/molxK	506.79	Joback Method
cpg	148.00	J/molxK	541.99	Joback Method
cpg	152.81	J/molxK	577.19	Joback Method
cpg	157.32	J/molxK	612.39	Joback Method
cpg	161.53	J/molxK	647.59	Joback Method
cpg	165.48	J/molxK	682.79	Joback Method
cpg	169.16	J/molxK	717.98	Joback Method
dvisc	0.0325628	Paxs	277.38	Joback Method
dvisc	0.0089704	Paxs	315.62	Joback Method

dvisc	0.0032651	Paxs	353.85	Joback Method
dvisc	0.0014474	Paxs	392.09	Joback Method
dvisc	0.0007414	Paxs	430.32	Joback Method
dvisc	0.0004236	Paxs	468.56	Joback Method
dvisc	0.0002633	Paxs	506.79	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C598801&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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