

Butyl iodoacetate

Inchi:	InChI=1S/C6H11IO2/c1-2-3-4-9-6(8)5-7/h2-5H2,1H3
InchiKey:	MPLKDWCVBIOQRN-UHFFFAOYSA-N
Formula:	C6H11IO2
SMILES:	CCCCOC(=O)CI
Mol. weight [g/mol]:	242.05

Physical Properties

Property code	Value	Unit	Source
gf	-176.16	kJ/mol	Joback Method
hf	-335.10	kJ/mol	Joback Method
hfus	18.49	kJ/mol	Joback Method
hvap	47.48	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	1.765		Crippen Method
mcvol	128.660	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
tb	506.11	K	Joback Method
tc	715.74	K	Joback Method
tf	287.60	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.54	J/molxK	506.11	Joback Method
cpg	255.51	J/molxK	541.05	Joback Method
cpg	264.99	J/molxK	575.99	Joback Method
cpg	274.01	J/molxK	610.93	Joback Method
cpg	282.57	J/molxK	645.86	Joback Method
cpg	290.68	J/molxK	680.80	Joback Method
cpg	298.35	J/molxK	715.74	Joback Method
dvisc	0.0035969	Paxs	287.60	Joback Method
dvisc	0.0019254	Paxs	324.02	Joback Method
dvisc	0.0011694	Paxs	360.44	Joback Method

dvisc	0.0007783	Paxs	396.86	Joback Method
dvisc	0.0005547	Paxs	433.27	Joback Method
dvisc	0.0004167	Paxs	469.69	Joback Method
dvisc	0.0003261	Paxs	506.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R248298&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

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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