Octyl iodoacetate

Inchi: InChI=1S/C10H19IO2/c1-2-3-4-5-6-7-8-13-10(12)9-11/h2-9H2,1H3
InchiKey: PTMGITASNQPNJJ-UHFFFAOYSA-N
Formula: C10H19IO2
SMILES: CCCCCCCCOC(=O)CI
Mol. weight [g/mol]: 298.16

Physical Properties

Property code	Value	Unit	Source
gf	-142.48	kJ/mol	Joback Method
hf	-417.66	kJ/mol	Joback Method
hfus	28.85	kJ/mol	Joback Method
hvap	56.38	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.325		Crippen Method
mcvol	185.020	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
rinpol	1581.20		NIST Webbook
tb	597.63	K	Joback Method
tc	795.28	K	Joback Method
tf	332.68	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.54	J/mol×K	597.63	Joback Method
cpg	440.27	J/mol×K	630.57	Joback Method
cpg	453.33	J/mol×K	663.51	Joback Method
cpg	465.72	J/mol×K	696.45	Joback Method
cpg	477.47	J/mol×K	729.39	Joback Method
cpg	488.59	J/mol×K	762.34	Joback Method
cpg	499.11	J/mol×K	795.28	Joback Method
dvisc	0.0029191	Pa×s	332.68	Joback Method
dvisc	0.0014555	Pa×s	376.84	Joback Method

dvisc	0.0008398	Pa×s	421.00	Joback Method
dvisc	0.0005379	Pa×s	465.15	Joback Method
dvisc	0.0003722	Pa×s	509.31	Joback Method
dvisc	0.0002731	Pa×s	553.47	Joback Method
dvisc	0.0002098	Pa×s	597.63	Joback Method

Sources

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=R248387&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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