

Nonyl iodoacetate

Inchi:	InChI=1S/C11H21IO2/c1-2-3-4-5-6-7-8-9-14-11(13)10-12/h2-10H2,1H3
InchiKey:	IKPAMRQMGQGHLX-UHFFFAOYSA-N
Formula:	C11H21IO2
SMILES:	CCCCCCCCCOC(=O)CI
Mol. weight [g/mol]:	312.19

Physical Properties

Property code	Value	Unit	Source
gf	-134.06	kJ/mol	Joback Method
hf	-438.30	kJ/mol	Joback Method
hfus	31.44	kJ/mol	Joback Method
hvap	58.61	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.715		Crippen Method
mvol	199.110	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
rinpol	1681.30		NIST Webbook
rinpol	1681.30		NIST Webbook
tb	620.51	K	Joback Method
tc	815.62	K	Joback Method
tf	343.95	K	Joback Method
vc	0.763	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.09	J/molxK	620.51	Joback Method
cpg	490.49	J/molxK	653.03	Joback Method
cpg	504.17	J/molxK	685.55	Joback Method
cpg	517.16	J/molxK	718.07	Joback Method
cpg	529.48	J/molxK	750.59	Joback Method
cpg	541.13	J/molxK	783.11	Joback Method
cpg	552.15	J/molxK	815.62	Joback Method
dvisc	0.0027112	Paxs	343.95	Joback Method

dvisc	0.0013314	Paxs	390.04	Joback Method
dvisc	0.0007598	Paxs	436.14	Joback Method
dvisc	0.0004827	Paxs	482.23	Joback Method
dvisc	0.0003320	Paxs	528.32	Joback Method
dvisc	0.0002424	Paxs	574.42	Joback Method
dvisc	0.0001855	Paxs	620.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R248372&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

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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