

Propionic acid, 3-iodo-, hexyl ester

Inchi:	InChI=1S/C9H17IO2/c1-2-3-4-5-8-12-9(11)6-7-10/h2-8H2,1H3
InchiKey:	PNZVARIWXDPJLC-UHFFFAOYSA-N
Formula:	C9H17IO2
SMILES:	CCCCCOC(=O)CCI
Mol. weight [g/mol]:	284.13

Physical Properties

Property code	Value	Unit	Source
gf	-150.90	kJ/mol	Joback Method
hf	-397.02	kJ/mol	Joback Method
hfus	26.26	kJ/mol	Joback Method
hvap	54.16	kJ/mol	Joback Method
log10ws	-3.40		Crippen Method
logp	2.935		Crippen Method
mcvol	170.930	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
rinpol	1527.00		NIST Webbook
rinpol	1527.00		NIST Webbook
tb	574.75	K	Joback Method
tc	775.16	K	Joback Method
tf	321.41	K	Joback Method
vc	0.651	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.61	J/molxK	574.75	Joback Method
cpg	437.23	J/molxK	741.76	Joback Method
cpg	426.72	J/molxK	708.36	Joback Method
cpg	415.62	J/molxK	674.96	Joback Method
cpg	403.91	J/molxK	641.55	Joback Method
cpg	391.58	J/molxK	608.15	Joback Method
cpg	447.17	J/molxK	775.16	Joback Method
dvisc	0.0002362	Paxs	574.75	Joback Method

dvisc	0.0003062	Paxs	532.53	Joback Method
dvisc	0.0004151	Paxs	490.30	Joback Method
dvisc	0.0005960	Paxs	448.08	Joback Method
dvisc	0.0009225	Paxs	405.86	Joback Method
dvisc	0.0015803	Paxs	363.63	Joback Method
dvisc	0.0031185	Paxs	321.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406241&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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