

Decanoic acid, 2-iodoethyl ester

Inchi:	InChI=1S/C12H23IO2/c1-2-3-4-5-6-7-8-9-12(14)15-11-10-13/h2-11H2,1H3
InchiKey:	TWESIZITODSXKE-UHFFFAOYSA-N
Formula:	C12H23IO2
SMILES:	CCCCCCCCC(=O)OCCI
Mol. weight [g/mol]:	326.21

Physical Properties

Property code	Value	Unit	Source
gf	-125.64	kJ/mol	Joback Method
hf	-458.94	kJ/mol	Joback Method
hfus	34.03	kJ/mol	Joback Method
hvap	60.83	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	4.105		Crippen Method
mcvol	213.200	ml/mol	McGowan Method
pc	1816.95	kPa	Joback Method
rinqol	1784.00		NIST Webbook
tb	643.39	K	Joback Method
tc	836.26	K	Joback Method
tf	355.22	K	Joback Method
vc	0.820	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.16	J/molxK	643.39	Joback Method
cpg	594.81	J/molxK	804.11	Joback Method
cpg	582.69	J/molxK	771.97	Joback Method
cpg	569.89	J/molxK	739.82	Joback Method
cpg	556.38	J/molxK	707.68	Joback Method
cpg	542.15	J/molxK	675.53	Joback Method
cpg	606.27	J/molxK	836.26	Joback Method
dvisc	0.0001633	Paxs	643.39	Joback Method
dvisc	0.0002142	Paxs	595.36	Joback Method

dvisc	0.0002947	Paxs	547.33	Joback Method
dvisc	0.0004310	Paxs	499.30	Joback Method
dvisc	0.0006837	Paxs	451.28	Joback Method
dvisc	0.0012103	Paxs	403.25	Joback Method
dvisc	0.0025005	Paxs	355.22	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=R19886&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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