

Octanoic acid, 2-iodoethyl ester

Inchi:	InChI=1S/C10H19IO2/c1-2-3-4-5-6-7-10(12)13-9-8-11/h2-9H2,1H3
InchiKey:	OYCNZICUZGYPJK-UHFFFAOYSA-N
Formula:	C10H19IO2
SMILES:	CCCCCCCC(=O)OCCI
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
mvol	185.020	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
rinpol	1583.00		NIST Webbook
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tb	597.63	K	Joback Method
tc	795.28	K	Joback Method
tf	332.68	K	Joback Method
vc	0.708	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.54	J/molxK	597.63	Joback Method
cpg	440.27	J/molxK	630.57	Joback Method
cpg	453.33	J/molxK	663.51	Joback Method
cpg	465.72	J/molxK	696.45	Joback Method
cpg	477.47	J/molxK	729.39	Joback Method
cpg	488.59	J/molxK	762.34	Joback Method
cpg	499.11	J/molxK	795.28	Joback Method
dvisc	0.0029191	Paxs	332.68	Joback Method

dvisc	0.0014555	Paxs	376.84	Joback Method
dvisc	0.0008398	Paxs	421.00	Joback Method
dvisc	0.0005379	Paxs	465.15	Joback Method
dvisc	0.0003722	Paxs	509.31	Joback Method
dvisc	0.0002731	Paxs	553.47	Joback Method
dvisc	0.0002098	Paxs	597.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R19989&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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