

Propionic acid, 3-iodo-, tetradecyl ester

Inchi:	InChI=1S/C17H33IO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-20-17(19)14-15-18/h2-16H2,1H
InchiKey:	ASZJONDGXFMEQA-UHFFFAOYSA-N
Formula:	C17H33IO2
SMILES:	CCCCCCCCCCCCCOC(=O)CCI
Mol. weight [g/mol]:	396.35

Physical Properties

Property code	Value	Unit	Source
gf	-83.54	kJ/mol	Joback Method
hf	-562.14	kJ/mol	Joback Method
hfus	46.98	kJ/mol	Joback Method
hvap	71.97	kJ/mol	Joback Method
log10ws	-6.75		Crippen Method
logp	6.056		Crippen Method
mvol	283.650	ml/mol	McGowan Method
pc	1252.15	kPa	Joback Method
rinpol	2363.00		NIST Webbook
rinpol	2363.00		NIST Webbook
tb	757.79	K	Joback Method
tc	945.34	K	Joback Method
tf	411.57	K	Joback Method
vc	1.099	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	802.24	J/molxK	757.79	Joback Method
cpg	819.35	J/molxK	789.05	Joback Method
cpg	835.58	J/molxK	820.31	Joback Method
cpg	850.94	J/molxK	851.57	Joback Method
cpg	865.47	J/molxK	882.83	Joback Method
cpg	879.20	J/molxK	914.08	Joback Method
cpg	892.16	J/molxK	945.34	Joback Method
dvisc	0.0015312	Paxs	411.57	Joback Method

dvisc	0.0006969	Paxs	469.27	Joback Method
dvisc	0.0003768	Paxs	526.98	Joback Method
dvisc	0.0002301	Paxs	584.68	Joback Method
dvisc	0.0001535	Paxs	642.38	Joback Method
dvisc	0.0001094	Paxs	700.09	Joback Method
dvisc	0.0000822	Paxs	757.79	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406245&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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