Propionic acid, 3-iodo-, tridecyl ester

Inchi: InChI=1S/C16H31IO2/c1-2-3-4-5-6-7-8-9-10-11-12-15-19-16(18)13-14-17/h2-15H2,1H3
InchiKey: ADHQYZDCEIWAOQ-UHFFFAOYSA-N
Formula: C16H31IO2
SMILES: CCCCCCCCCCCCCOC(=O)CCI
Mol. weight [g/mol]: 382.32

Physical Properties

Property code	Value	Unit	Source
gf	-91.96	kJ/mol	Joback Method
hf	-541.50	kJ/mol	Joback Method
hfus	44.39	kJ/mol	Joback Method
hvap	69.74	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	5.666		Crippen Method
mcvol	269.560	ml/mol	McGowan Method
pc	1341.76	kPa	Joback Method
rinpol	2258.00		NIST Webbook
tb	734.91	K	Joback Method
tc	922.58	K	Joback Method
tf	400.30	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.87	J/mol×K	734.91	Joback Method
cpg	761.63	J/mol×K	766.19	Joback Method
cpg	777.52	J/mol×K	797.47	Joback Method
cpg	792.58	J/mol×K	828.74	Joback Method
cpg	806.83	J/mol×K	860.02	Joback Method
cpg	820.30	J/mol×K	891.30	Joback Method
cpg	833.02	J/mol×K	922.58	Joback Method
dvisc	0.0017058	Pa×s	400.30	Joback Method
dvisc	0.0007850	Pa×s	456.07	Joback Method

dvisc	0.0004278	Pa×s	511.84	Joback Method
dvisc	0.0002627	Pa×s	567.61	Joback Method
dvisc	0.0001760	Pa×s	623.37	Joback Method
dvisc	0.0001259	Pa×s	679.14	Joback Method
dvisc	0.0000948	Pa×s	734.91	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=U406244&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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