Propionic acid, 3-iodo-, octadecyl ester

Inchi: InChI=1S/C21H41IO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-24-21(23)18-19-2
InchiKey: XOHCTGSZYYCPOD-UHFFFAOYSA-N
Formula: C21H41IO2
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCI
Mol. weight [g/mol]: 452.45

Physical Properties

Property code	Value	Unit	Source
gf	-49.86	kJ/mol	Joback Method
hf	-644.70	kJ/mol	Joback Method
hfus	57.34	kJ/mol	Joback Method
hvap	80.87	kJ/mol	Joback Method
log10ws	-8.42		Crippen Method
logp	7.616		Crippen Method
mcvol	340.010	ml/mol	McGowan Method
pc	970.49	kPa	Joback Method
rinpol	2785.00		NIST Webbook
tb	849.31	K	Joback Method
tc	1042.70	K	Joback Method
tf	456.65	K	Joback Method
vc	1.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1041.16	J/mol×K	849.31	Joback Method
cpg	1124.10	J/mol×K	1010.47	Joback Method
cpg	1109.42	J/mol×K	978.24	Joback Method
cpg	1093.84	J/mol×K	946.00	Joback Method
cpg	1077.30	J/mol×K	913.77	Joback Method
cpg	1059.75	J/mol×K	881.54	Joback Method
cpg	1137.90	J/mol×K	1042.70	Joback Method
dvisc	0.0000453	Pa×s	849.31	Joback Method
dvisc	0.0000610	Pa×s	783.87	Joback Method

dvisc	0.0000865	Pa×s	718.42	Joback Method
dvisc	0.0001316	Pa×s	652.98	Joback Method
dvisc	0.0002200	Pa×s	587.54	Joback Method
dvisc	0.0004184	Pa×s	522.09	Joback Method
dvisc	0.0009562	Pa×s	456.65	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U406249&Units=SI

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