Propionic acid, 3-iodo-, hexadecyl ester

Inchi: InChI=1S/C19H37IO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-22-19(21)16-17-20/h2-1
InchiKey: AMBMHTVKDPBYIM-UHFFFAOYSA-N
Formula: C19H37IO2
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCI
Mol. weight [g/mol]: 424.40

Physical Properties

Property code	Value	Unit	Source
gf	-66.70	kJ/mol	Joback Method
hf	-603.42	kJ/mol	Joback Method
hfus	52.16	kJ/mol	Joback Method
hvap	76.42	kJ/mol	Joback Method
log10ws	-7.59		Crippen Method
logp	6.836		Crippen Method
mcvol	311.830	ml/mol	McGowan Method
pc	1097.90	kPa	Joback Method
rinpol	2578.00		NIST Webbook
rinpol	2578.00		NIST Webbook
tb	803.55	K	Joback Method
tc	992.65	K	Joback Method
tf	434.11	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	919.94	J/mol×K	803.55	Joback Method
cpg	999.85	J/mol×K	961.14	Joback Method
cpg	985.65	J/mol×K	929.62	Joback Method
cpg	970.59	J/mol×K	898.10	Joback Method
cpg	954.64	J/mol×K	866.58	Joback Method
cpg	937.77	J/mol×K	835.07	Joback Method
cpg	1013.24	J/mol×K	992.65	Joback Method
dvisc	0.0000613	Pa×s	803.55	Joback Method

dvisc	0.0000820	Pa×s	741.98	Joback Method
dvisc	0.0001158	Pa×s	680.40	Joback Method
dvisc	0.0001749	Pa×s	618.83	Joback Method
dvisc	0.0002896	Pa×s	557.26	Joback Method
dvisc	0.0005433	Pa×s	495.68	Joback Method
dvisc	0.0012187	Pa×s	434.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406247&Units=SI
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

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