Propionic acid, 3-iodo-, pentadecyl ester

Inchi: InChI=1S/C18H35IO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-21-18(20)15-16-19/h2-17H2
InchiKey: LMLSJCYHMQXXQW-UHFFFAOYSA-N
Formula: C18H35IO2
SMILES: CCCCCCCCCCCCCCCOC(=O)CCI
Mol. weight [g/mol]: 410.37

Physical Properties

Property code	Value	Unit	Source
gf	-75.12	kJ/mol	Joback Method
hf	-582.78	kJ/mol	Joback Method
hfus	49.57	kJ/mol	Joback Method
hvap	74.19	kJ/mol	Joback Method
log10ws	-7.17		Crippen Method
logp	6.446		Crippen Method
mcvol	297.740	ml/mol	McGowan Method
pc	1171.22	kPa	Joback Method
rinpol	2471.00		NIST Webbook
tb	780.67	K	Joback Method
tc	968.69	K	Joback Method
tf	422.84	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	860.62	J/mol×K	780.67	Joback Method
cpg	878.09	J/mol×K	812.01	Joback Method
cpg	894.64	J/mol×K	843.34	Joback Method
cpg	910.29	J/mol×K	874.68	Joback Method
cpg	925.09	J/mol×K	906.01	Joback Method
cpg	939.06	J/mol×K	937.35	Joback Method
cpg	952.24	J/mol×K	968.69	Joback Method
dvisc	0.0013687	Pa×s	422.84	Joback Method
dvisc	0.0006164	Pa×s	482.48	Joback Method

dvisc	0.0003308	Pa×s	542.12	Joback Method
dvisc	0.0002009	Pa×s	601.75	Joback Method
dvisc	0.0001335	Pa×s	661.39	Joback Method
dvisc	0.0000949	Pa×s	721.03	Joback Method
dvisc	0.0000710	Pa×s	780.67	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=U406246&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