Propionic acid, 3-iodo-, heptadecyl ester

Inchi: InChI=1S/C20H39IO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-23-20(22)17-18-21/h
InchiKey: QCXRMVWNLJPIFE-UHFFFAOYSA-N
Formula: C20H39IO2
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCI
Mol. weight [g/mol]: 438.43

Physical Properties

Property code	Value	Unit	Source
gf	-58.28	kJ/mol	Joback Method
hf	-624.06	kJ/mol	Joback Method
hfus	54.75	kJ/mol	Joback Method
hvap	78.64	kJ/mol	Joback Method
log10ws	-8.01		Crippen Method
logp	7.226		Crippen Method
mcvol	325.920	ml/mol	McGowan Method
pc	1031.25	kPa	Joback Method
rinpol	2684.00		NIST Webbook
tb	826.43	K	Joback Method
tc	1017.31	K	Joback Method
tf	445.38	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.15	J/mol×K	826.43	Joback Method
cpg	1061.54	J/mol×K	985.49	Joback Method
cpg	1047.10	J/mol×K	953.68	Joback Method
cpg	1031.78	J/mol×K	921.87	Joback Method
cpg	1015.54	J/mol×K	890.06	Joback Method
cpg	998.35	J/mol×K	858.24	Joback Method
cpg	1075.13	J/mol×K	1017.31	Joback Method
dvisc	0.0000528	Pa×s	826.43	Joback Method
dvisc	0.0000708	Pa×s	762.92	Joback Method

dvisc	0.0001002	Pa×s	699.41	Joback Method
dvisc	0.0001519	Pa×s	635.90	Joback Method
dvisc	0.0002528	Pa×s	572.40	Joback Method
dvisc	0.0004775	Pa×s	508.89	Joback Method
dvisc	0.0010813	Pa×s	445.38	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=U406248&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