Propanoic acid, octadecyl ester

Other names: Octadecyl propionate
Inchi: InChI=1S/C21H42O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-21(22)4-2/h3
InchiKey: YTXCAJNHPVBVDJ-UHFFFAOYSA-N
Formula: C21H42O2
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CC
Mol. weight [g/mol]: 326.56

Physical Properties

Property code	Value	Unit	Source
gf	-107.98	kJ/mol	Joback Method
hf	-721.57	kJ/mol	Joback Method
hfus	52.93	kJ/mol	Joback Method
hvap	71.50	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	7.201		Crippen Method
mcvol	314.190	ml/mol	McGowan Method
pc	983.93	kPa	Joback Method
rinpol	2285.00		NIST Webbook
rinpol	2285.00		NIST Webbook
rinpol	2278.00		NIST Webbook
rinpol	2278.00		NIST Webbook
rinpol	2281.00		NIST Webbook
rinpol	2291.00		NIST Webbook
rinpol	2291.00		NIST Webbook
rinpol	2262.00		NIST Webbook
ripol	2550.00		NIST Webbook
ripol	2560.00		NIST Webbook
ripol	2577.00		NIST Webbook
ripol	2574.00		NIST Webbook
ripol	2570.00		NIST Webbook
ripol	2550.00		NIST Webbook
tb	756.17	K	Joback Method
tc	929.77	K	Joback Method
tf	398.59	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.32	J/mol×K	756.17	Joback Method
cpg	1060.46	J/mol×K	900.83	Joback Method
cpg	1044.06	J/mol×K	871.90	Joback Method
cpg	1026.77	J/mol×K	842.97	Joback Method
cpg	1008.57	J/mol×K	814.04	Joback Method
cpg	989.43	J/mol×K	785.10	Joback Method
cpg	1075.99	J/mol×K	929.77	Joback Method
dvisc	0.0000640	Pa×s	756.17	Joback Method
dvisc	0.0000864	Pa×s	696.57	Joback Method
dvisc	0.0001235	Pa×s	636.98	Joback Method
dvisc	0.0001899	Pa×s	577.38	Joback Method
dvisc	0.0003224	Pa×s	517.78	Joback Method
dvisc	0.0006283	Pa×s	458.19	Joback Method
dvisc	0.0014949	Pa×s	398.59	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=R23871&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume