2-Propenoic acid, tetradecyl ester

Other names: 2-Propenoic acid, n-tetradecyl ester
Tetradecyl acrylate
Inchi: InChI=1S/C17H32O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-19-17(18)4-2/h4H,2-3,5-16H
InchiKey: XZHNPVKXBNDGJD-UHFFFAOYSA-N
Formula: C17H32O2
SMILES: C=CC(=O)OCCCCCCCCCCCCCC
Mol. weight [g/mol]: 268.43
CAS: 21643-42-5

Physical Properties

Property code	Value	Unit	Source
gf	-53.82	kJ/mol	Joback Method
hf	-513.58	kJ/mol	Joback Method
hfus	41.29	kJ/mol	Joback Method
hvap	61.92	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.417		Crippen Method
mcvol	253.530	ml/mol	McGowan Method
pc	1310.85	kPa	Joback Method
rinpol	1876.00		NIST Webbook
ripol	2201.00		NIST Webbook
ripol	2201.00		NIST Webbook
tb	661.33	K	Joback Method
tc	830.65	K	Joback Method
tf	287.00 ± 3.00	K	NIST Webbook
vc	0.993	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.54	J/mol×K	830.65	Joback Method
cpg	790.43	J/mol×K	802.43	Joback Method
cpg	775.61	J/mol×K	774.21	Joback Method
cpg	760.05	J/mol×K	745.99	Joback Method

cpg	743.76	J/mol×K	717.77	Joback Method
cpg	726.69	J/mol×K	689.55	Joback Method
cpg	708.83	J/mol×K	661.33	Joback Method
dvisc	0.0021607	Pa×s	351.75	Joback Method
dvisc	0.0001135	Pa×s	661.33	Joback Method
dvisc	0.0001506	Pa×s	609.73	Joback Method
dvisc	0.0002107	Pa×s	558.14	Joback Method
dvisc	0.0003156	Pa×s	506.54	Joback Method
dvisc	0.0005182	Pa×s	454.94	Joback Method
dvisc	0.0009658	Pa×s	403.35	Joback Method
hvapt	69.40	kJ/mol	529.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21643425&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

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
hvapt: Enthalpy of vaporization at a given temperature
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