ACETIC ACID, 3,7,11,15-TETRAMETHYL-HEXADECYL ESTER

Other names: 3,7,11,15-Tetramethyl-hexadecyl acetate
Inchi: InChI=1S/C22H44O2/c1-18(2)10-7-11-19(3)12-8-13-20(4)14-9-15-21(5)16-17-24-22(6)23
InchiKey: QSEOJZDSLREMLU-UHFFFAOYSA-N
Formula: C22H44O2
SMILES: CC(=O)OCCC(C)CCCC(C)CCCC(C)CCCC(C)C
Mol. weight [g/mol]: 340.59

Physical Properties

Property code	Value	Unit	Source
af	0.8684		Cheméo Relay (1.0)
hf	-891.15	kJ/mol	Cheméo Relay (1.0)
hfus	41.43	kJ/mol	Joback Method
hvap	103.27	kJ/mol	Cheméo Relay (1.0)
ie	9.39	eV	Cheméo Relay (1.0)
log10ws	-7.29		Cheméo Relay (1.0)
logp	7.015		Crippen Method
mcvol	328.280	ml/mol	McGowan Method
pc	945.58	kPa	Joback Method
tb	606.73	K	Cheméo Relay (1.0)
tc	772.81	K	Cheméo Relay (1.0)
tf	242.21	K	Cheméo Relay (1.0)
vc	1.219	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1032.75	J/mol×K	777.29	Joback Method
cpg	1053.78	J/mol×K	807.29	Joback Method
cpg	1073.71	J/mol×K	837.29	Joback Method
cpg	1092.57	J/mol×K	867.29	Joback Method
cpg	1110.40	J/mol×K	897.30	Joback Method
cpg	1127.22	J/mol×K	927.30	Joback Method
cpg	1143.07	J/mol×K	957.30	Joback Method
dvisc	0.0038145	Pa×s	349.86	Joback Method

dvisc	0.0009378	Pa×s	421.10	Joback Method
dvisc	0.0003460	Pa×s	492.34	Joback Method
dvisc	0.0001643	Pa×s	563.58	Joback Method
dvisc	0.0000922	Pa×s	634.81	Joback Method
dvisc	0.0000581	Pa×s	706.05	Joback Method
dvisc	0.0000399	Pa×s	777.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U193630&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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