Hexanoic acid, 3,5,5-trimethyl-, dodecyl ester

Inchi: InChI=1S/C21H42O2/c1-6-7-8-9-10-11-12-13-14-15-16-23-20(22)17-19(2)18-21(3,4)5/h1
InchiKey: XVDCXGOGHRIMJF-UHFFFAOYSA-N
Formula: C21H42O2
SMILES: CCCCCCCCCCCCOC(=O)CC(C)CC(C)(C)C
Mol. weight [g/mol]: 326.56

Physical Properties

Property code	Value	Unit	Source
gf	-107.58	kJ/mol	Joback Method
hf	-735.60	kJ/mol	Joback Method
hfus	42.00	kJ/mol	Joback Method
hvap	69.81	kJ/mol	Joback Method
log10ws	-6.99		Crippen Method
logp	6.913		Crippen Method
mcvol	314.190	ml/mol	McGowan Method
pc	1000.81	kPa	Joback Method
rinpol	2139.00		NIST Webbook
rinpol	2139.00		NIST Webbook
tb	752.50	K	Joback Method
tc	930.17	K	Joback Method
tf	386.01	K	Joback Method
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.02	J/mol×K	752.50	Joback Method
cpg	991.40	J/mol×K	782.11	Joback Method
cpg	1010.75	J/mol×K	811.72	Joback Method
cpg	1029.12	J/mol×K	841.34	Joback Method
cpg	1046.53	J/mol×K	870.95	Joback Method
cpg	1063.03	J/mol×K	900.56	Joback Method
cpg	1078.66	J/mol×K	930.17	Joback Method
dvisc	0.0019589	Pa×s	386.01	Joback Method

dvisc	0.0006934	Pa×s	447.09	Joback Method
dvisc	0.0003150	Pa×s	508.17	Joback Method
dvisc	0.0001695	Pa×s	569.25	Joback Method
dvisc	0.0001029	Pa×s	630.34	Joback Method
dvisc	0.0000682	Pa×s	691.42	Joback Method
dvisc	0.0000483	Pa×s	752.50	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U406063&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
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