Octanoic acid, hexadecyl ester

Other names: hexadecyl octanoate
hexadecyl caprylate
Inchi: InChI=1S/C24H48O2/c1-3-5-7-9-10-11-12-13-14-15-16-17-19-21-23-26-24(25)22-20-18-
InchiKey: DWMMZQMXUWUJME-UHFFFAOYSA-N
Formula: C24H48O2
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCCCCC
Mol. weight [g/mol]: 368.64
CAS: 29710-31-4

Physical Properties

Property code	Value	Unit	Source
gf	-82.72	kJ/mol	Joback Method
hf	-783.49	kJ/mol	Joback Method
hfus	60.70	kJ/mol	Joback Method
hvap	78.17	kJ/mol	Joback Method
log10ws	-8.73		Crippen Method
logp	8.371		Crippen Method
mcvol	356.460	ml/mol	McGowan Method
pc	827.64	kPa	Joback Method
rinpol	2576.30		NIST Webbook
rinpol	2576.30		NIST Webbook
rinpol	2562.00		NIST Webbook
rinpol	2562.00		NIST Webbook
tb	824.81	K	Joback Method
tc	1009.81	K	Joback Method
tf	432.40	K	Joback Method
vc	1.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1156.81	J/mol×K	824.81	Joback Method
cpg	1178.47	J/mol×K	855.64	Joback Method
cpg	1198.97	J/mol×K	886.48	Joback Method

cpg	1218.34	J/mol×K	917.31	Joback Method
cpg	1236.63	J/mol×K	948.14	Joback Method
cpg	1253.86	J/mol×K	978.97	Joback Method
cpg	1270.08	J/mol×K	1009.81	Joback Method
dvisc	0.0010603	Pa×s	432.40	Joback Method
dvisc	0.0004342	Pa×s	497.80	Joback Method
dvisc	0.0002188	Pa×s	563.20	Joback Method
dvisc	0.0001271	Pa×s	628.61	Joback Method
dvisc	0.0000818	Pa×s	694.01	Joback Method
dvisc	0.0000568	Pa×s	759.41	Joback Method
dvisc	0.0000418	Pa×s	824.81	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=C29710314&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume