Decanoic acid, hexyl ester

Other names: hexyl decanoate
Hexyl caprate
Inchi: InChI=1S/C16H32O2/c1-3-5-7-9-10-11-12-14-16(17)18-15-13-8-6-4-2/h3-15H2,1-2H3
InchiKey: DGPNTCACXCHFDI-UHFFFAOYSA-N
Formula: C16H32O2
SMILES: CCCCCCCCCC(=O)OCCCCCC
Mol. weight [g/mol]: 256.42
CAS: 10448-26-7

Physical Properties

Property code	Value	Unit	Source
gf	-150.08	kJ/mol	Joback Method
hf	-618.37	kJ/mol	Joback Method
hfus	39.98	kJ/mol	Joback Method
hvap	60.37	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	5.251		Crippen Method
mcvol	243.740	ml/mol	McGowan Method
pc	1363.65	kPa	Joback Method
rinpol	1783.80		NIST Webbook
rinpol	1763.00		NIST Webbook
rinpol	1784.00		NIST Webbook
rinpol	1784.00		NIST Webbook
rinpol	1783.80		NIST Webbook
ripol	2011.00		NIST Webbook
ripol	2017.00		NIST Webbook
ripol	1998.00		NIST Webbook
ripol	1998.00		NIST Webbook
ripol	2011.00		NIST Webbook
ripol	2017.00		NIST Webbook
tb	641.77	K	Joback Method
tc	809.14	K	Joback Method
tf	253.86 ± 1.50	K	NIST Webbook
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.85	J/mol×K	641.77	Joback Method
cpg	757.90	J/mol×K	781.24	Joback Method
cpg	742.94	J/mol×K	753.35	Joback Method
cpg	727.27	J/mol×K	725.45	Joback Method
cpg	710.87	J/mol×K	697.56	Joback Method
cpg	693.74	J/mol×K	669.66	Joback Method
cpg	772.16	J/mol×K	809.14	Joback Method
dvisc	0.0001221	Pa×s	641.77	Joback Method
dvisc	0.0001627	Pa×s	591.85	Joback Method
dvisc	0.0002286	Pa×s	541.93	Joback Method
dvisc	0.0003441	Pa×s	492.00	Joback Method
dvisc	0.0005682	Pa×s	442.08	Joback Method
dvisc	0.0010661	Pa×s	392.16	Joback Method
dvisc	0.0024033	Pa×s	342.24	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10448267&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume