

Hexanoic acid, decyl ester

Other names:	Decyl caproate decyl hexanoate
Inchi:	InChI=1S/C16H32O2/c1-3-5-7-8-9-10-11-13-15-18-16(17)14-12-6-4-2/h3-15H2,1-2H3
InchiKey:	QNKHVQVPARQEKZ-UHFFFAOYSA-N
Formula:	C16H32O2
SMILES:	CCCCCCCCCOC(=O)CCCCC
Mol. weight [g/mol]:	256.42
CAS:	52363-43-6

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
mvol	243.740	ml/mol	McGowan Method
pc	1363.65	kPa	Joback Method
rinpol	1765.00		NIST Webbook
tb	641.77	K	Joback Method
tc	809.14	K	Joback Method
tf	342.24	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.85	J/molxK	641.77	Joback Method
cpg	693.74	J/molxK	669.66	Joback Method
cpg	710.87	J/molxK	697.56	Joback Method
cpg	727.27	J/molxK	725.45	Joback Method
cpg	742.94	J/molxK	753.35	Joback Method
cpg	757.90	J/molxK	781.24	Joback Method

cpg	772.16	J/mol×K	809.14	Joback Method
dvisc	0.0024033	Paxs	342.24	Joback Method
dvisc	0.0010661	Paxs	392.16	Joback Method
dvisc	0.0005682	Paxs	442.08	Joback Method
dvisc	0.0003441	Paxs	492.00	Joback Method
dvisc	0.0002286	Paxs	541.93	Joback Method
dvisc	0.0001627	Paxs	591.85	Joback Method
dvisc	0.0001221	Paxs	641.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52363436&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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