

Hexanoic acid, hexadecyl ester

Other names:	Hexadecyl caproate
Inchi:	InChI=1S/C22H44O2/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-19-21-24-22(23)20-18-6-4-2
InchiKey:	SDPBXXCJVDQPIQ-UHFFFAOYSA-N
Formula:	C22H44O2
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCCC
Mol. weight [g/mol]:	340.58
CAS:	14331-11-4

Physical Properties

Property code	Value	Unit	Source
gf	-99.56	kJ/mol	Joback Method
hf	-742.21	kJ/mol	Joback Method
hfus	55.52	kJ/mol	Joback Method
hvap	73.72	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	7.591		Crippen Method
mcvol	328.280	ml/mol	McGowan Method
pc	927.24	kPa	Joback Method
rinpol	2366.00		NIST Webbook
rinpol	2366.00		NIST Webbook
tb	779.05	K	Joback Method
tc	955.69	K	Joback Method
tf	409.86	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.01	J/molxK	779.05	Joback Method
cpg	1051.60	J/molxK	808.49	Joback Method
cpg	1071.17	J/molxK	837.93	Joback Method
cpg	1089.74	J/molxK	867.37	Joback Method
cpg	1107.35	J/molxK	896.81	Joback Method
cpg	1124.02	J/molxK	926.25	Joback Method

cpg	1139.78	J/molxK	955.69	Joback Method
dvisc	0.0013386	Paxs	409.86	Joback Method
dvisc	0.0005575	Paxs	471.39	Joback Method
dvisc	0.0002843	Paxs	532.92	Joback Method
dvisc	0.0001666	Paxs	594.45	Joback Method
dvisc	0.0001080	Paxs	655.99	Joback Method
dvisc	0.0000754	Paxs	717.52	Joback Method
dvisc	0.0000557	Paxs	779.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14331114&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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