

3-Octenoic acid, hexadecyl ester

Inchi:	InChI=1S/C24H46O2/c1-3-5-7-9-10-11-12-13-14-15-16-17-19-21-23-26-24(25)22-20-18-
InchiKey:	MNVQHBRILWMBLM-CZIZESTLSA-N
Formula:	C24H46O2
SMILES:	CCCCC=CCC(=O)OCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	366.62

Physical Properties

Property code	Value	Unit	Source
gf	-2.50	kJ/mol	Joback Method
hf	-666.27	kJ/mol	Joback Method
hfus	60.90	kJ/mol	Joback Method
hvap	78.13	kJ/mol	Joback Method
log10ws	-8.58		Crippen Method
logp	8.147		Crippen Method
mvol	352.160	ml/mol	McGowan Method
pc	852.97	kPa	Joback Method
rinpol	2585.00		NIST Webbook
rinpol	2585.00		NIST Webbook
tb	828.97	K	Joback Method
tc	1015.16	K	Joback Method
tf	427.32	K	Joback Method
vc	1.383	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1131.61	J/molxK	828.97	Joback Method
cpg	1152.63	J/molxK	860.00	Joback Method
cpg	1172.54	J/molxK	891.03	Joback Method
cpg	1191.40	J/molxK	922.06	Joback Method
cpg	1209.26	J/molxK	953.09	Joback Method
cpg	1226.16	J/molxK	984.13	Joback Method
cpg	1242.15	J/molxK	1015.16	Joback Method
dvisc	0.0009923	Paxs	427.32	Joback Method

dvisc	0.0003939	Paxs	494.26	Joback Method
dvisc	0.0001949	Paxs	561.20	Joback Method
dvisc	0.0001121	Paxs	628.14	Joback Method
dvisc	0.0000717	Paxs	695.09	Joback Method
dvisc	0.0000496	Paxs	762.03	Joback Method
dvisc	0.0000364	Paxs	828.97	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
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=U406135&Units=SI

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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