

2-Heptenoic acid, tridecyl ester

Inchi: InChI=1S/C20H38O2/c1-3-5-7-9-10-11-12-13-14-15-17-19-22-20(21)18-16-8-6-4-2/h16,17,19,21,22
InchiKey: XLOGXVLKIOINOTI-FBMGVBCBSA-N
Formula: C20H38O2
SMILES: CCCCC=CC(=O)OCCCCCCCCCCCCC
Mol. weight [g/mol]: 310.51

Physical Properties

Property code	Value	Unit	Source
gf	-36.18	kJ/mol	Joback Method
hf	-583.71	kJ/mol	Joback Method
hfus	50.54	kJ/mol	Joback Method
hvap	69.23	kJ/mol	Joback Method
log10ws	-6.91		Crippen Method
logp	6.587		Crippen Method
mvol	295.800	ml/mol	McGowan Method
pc	1082.06	kPa	Joback Method
rinpol	2254.00		NIST Webbook
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tb	737.45	K	Joback Method
tc	911.93	K	Joback Method
tf	382.24	K	Joback Method
vc	1.159	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.45	J/molxK	737.45	Joback Method
cpg	904.58	J/molxK	766.53	Joback Method
cpg	922.81	J/molxK	795.61	Joback Method
cpg	940.17	J/molxK	824.69	Joback Method
cpg	956.69	J/molxK	853.77	Joback Method
cpg	972.40	J/molxK	882.85	Joback Method
cpg	987.32	J/molxK	911.93	Joback Method
dvisc	0.0015546	Paxs	382.24	Joback Method

dvisc	0.0006381	Paxs	441.44	Joback Method
dvisc	0.0003233	Paxs	500.64	Joback Method
dvisc	0.0001891	Paxs	559.84	Joback Method
dvisc	0.0001226	Paxs	619.05	Joback Method
dvisc	0.0000857	Paxs	678.25	Joback Method
dvisc	0.0000635	Paxs	737.45	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406098&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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