2-Heptenoic acid, octyl ester

Inchi: InChI=1S/C15H28O2/c1-3-5-7-9-10-12-14-17-15(16)13-11-8-6-4-2/h11,13H,3-10,12,14H
InchiKey: GGGUDHOEWILFKY-ACCUITESSA-N
Formula: C15H28O2
SMILES: CCCCC=CC(=O)OCCCCCCCC
Mol. weight [g/mol]: 240.38

Physical Properties

Property code	Value	Unit	Source
gf	-78.28	kJ/mol	Joback Method
hf	-480.51	kJ/mol	Joback Method
hfus	37.59	kJ/mol	Joback Method
hvap	58.10	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.636		Crippen Method
mcvol	225.350	ml/mol	McGowan Method
pc	1525.88	kPa	Joback Method
rinpol	1751.00		NIST Webbook
rinpol	1751.00		NIST Webbook
tb	623.05	K	Joback Method
tc	796.03	K	Joback Method
tf	325.89	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.59	J/mol×K	623.05	Joback Method
cpg	617.60	J/mol×K	651.88	Joback Method
cpg	633.86	J/mol×K	680.71	Joback Method
cpg	649.40	J/mol×K	709.54	Joback Method
cpg	664.23	J/mol×K	738.37	Joback Method
cpg	678.37	J/mol×K	767.20	Joback Method
cpg	691.85	J/mol×K	796.03	Joback Method
dvisc	0.0024199	Pa×s	325.89	Joback Method

dvisc	0.0010480	Pa×s	375.42	Joback Method
dvisc	0.0005516	Pa×s	424.94	Joback Method
dvisc	0.0003319	Pa×s	474.47	Joback Method
dvisc	0.0002199	Pa×s	524.00	Joback Method
dvisc	0.0001564	Pa×s	573.52	Joback Method
dvisc	0.0001174	Pa×s	623.05	Joback Method

Sources

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=U406094&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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